

FIG. 1(a)

09866543 - 052500

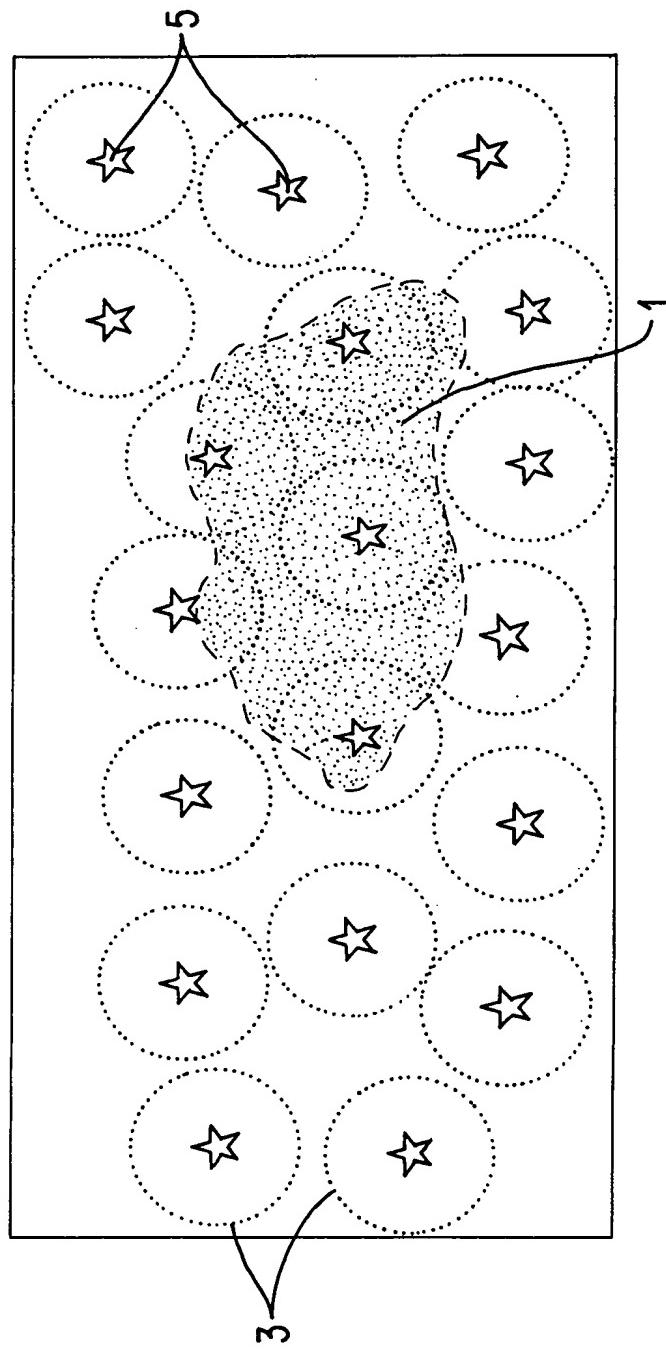


FIG. 1(b)

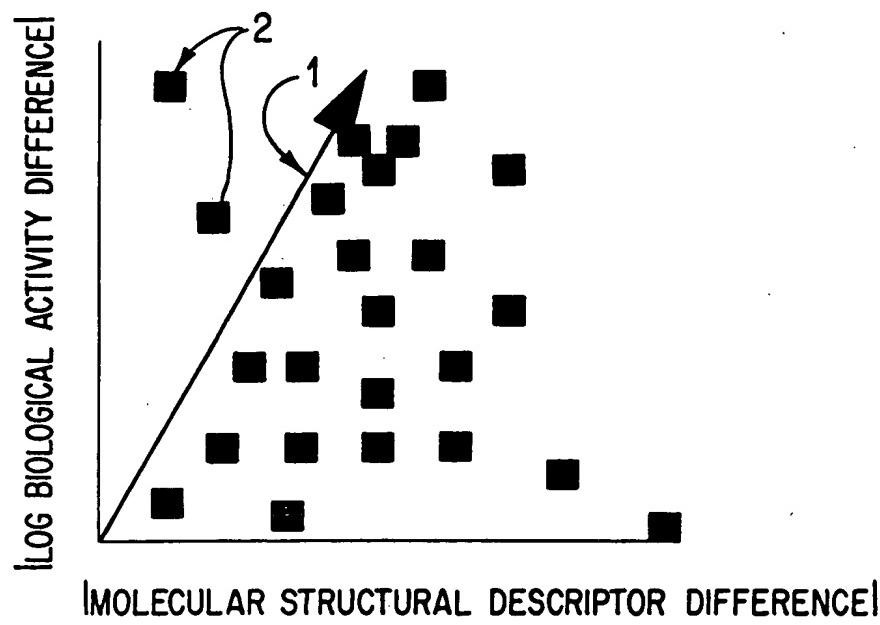


FIG. 2

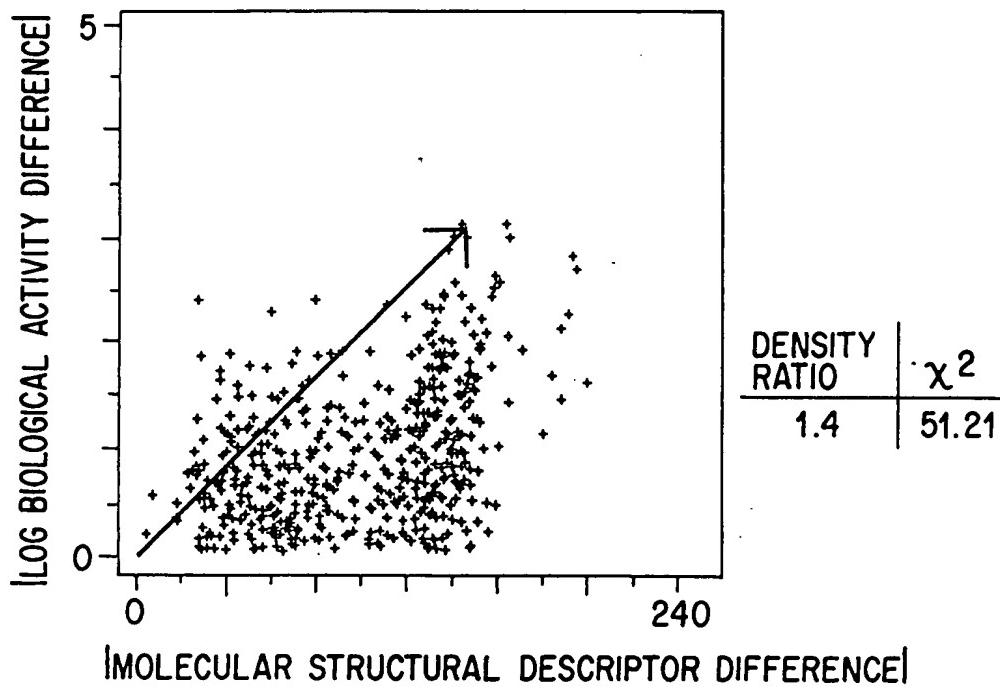


FIG. 3

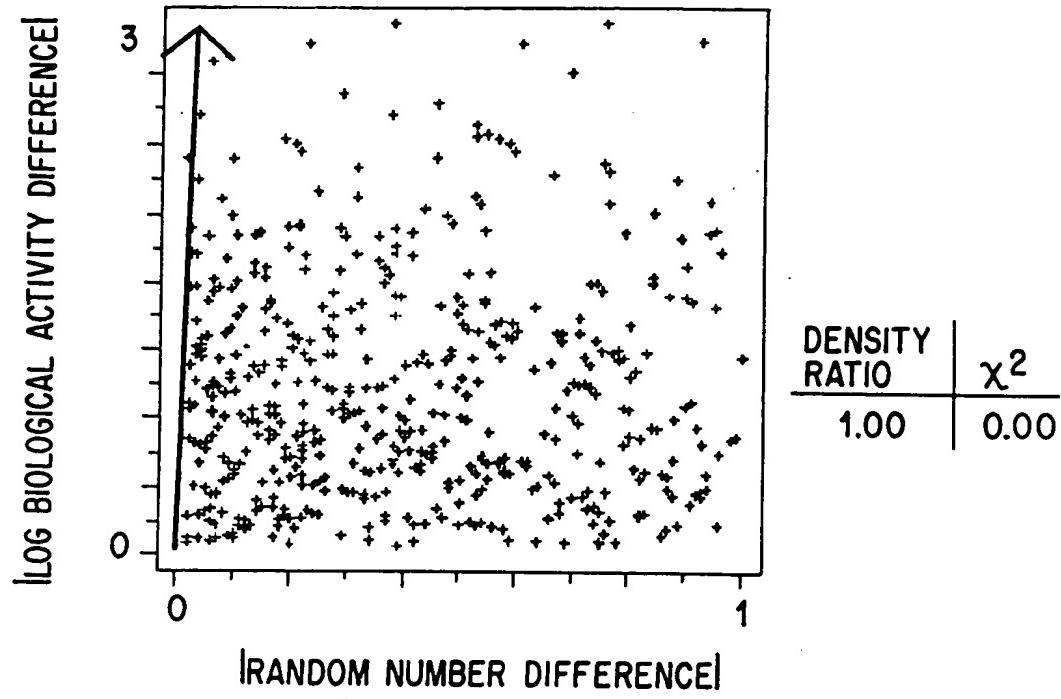


FIG. 4

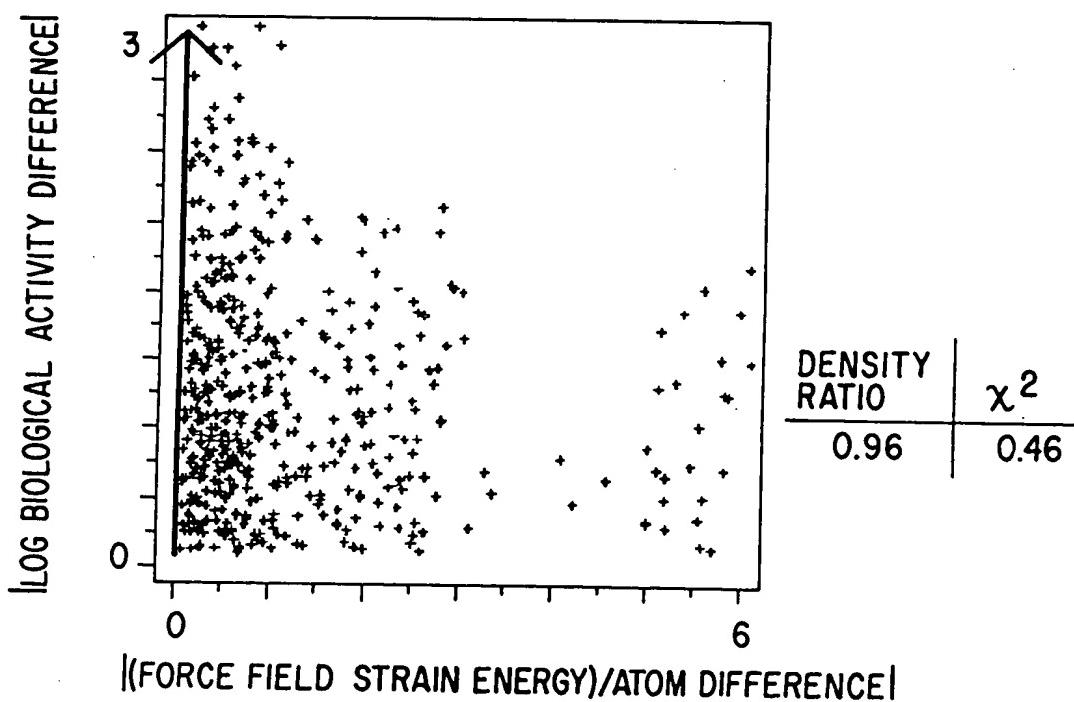
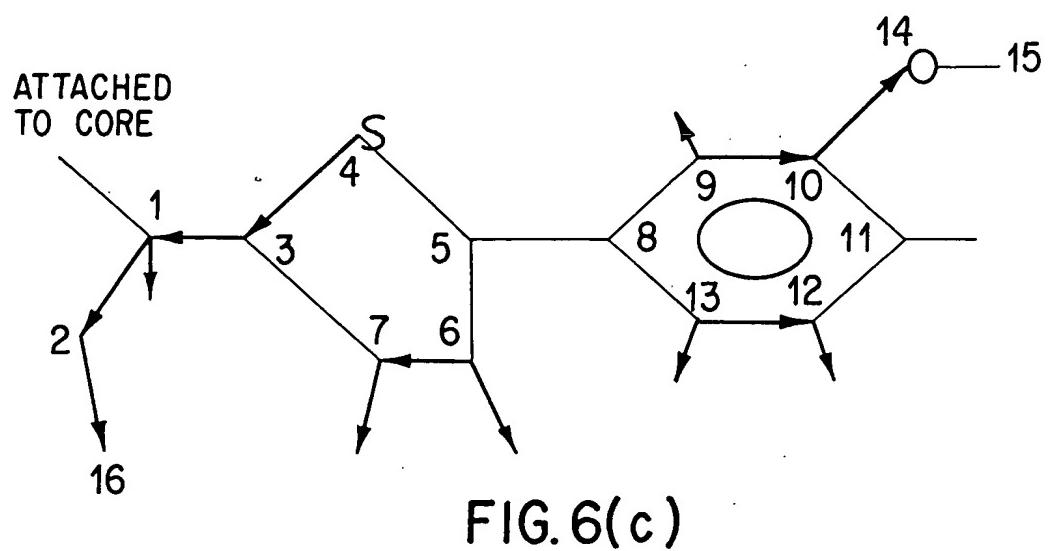
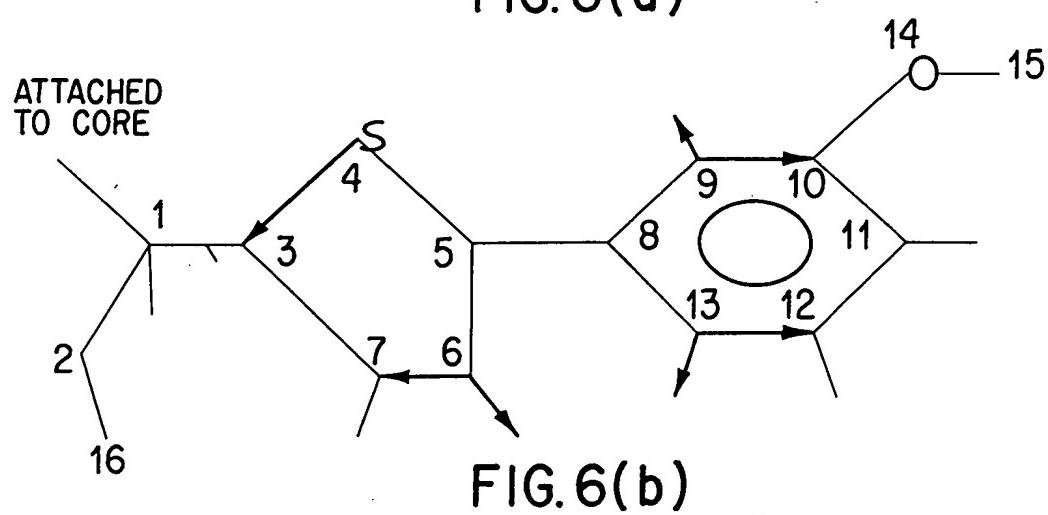
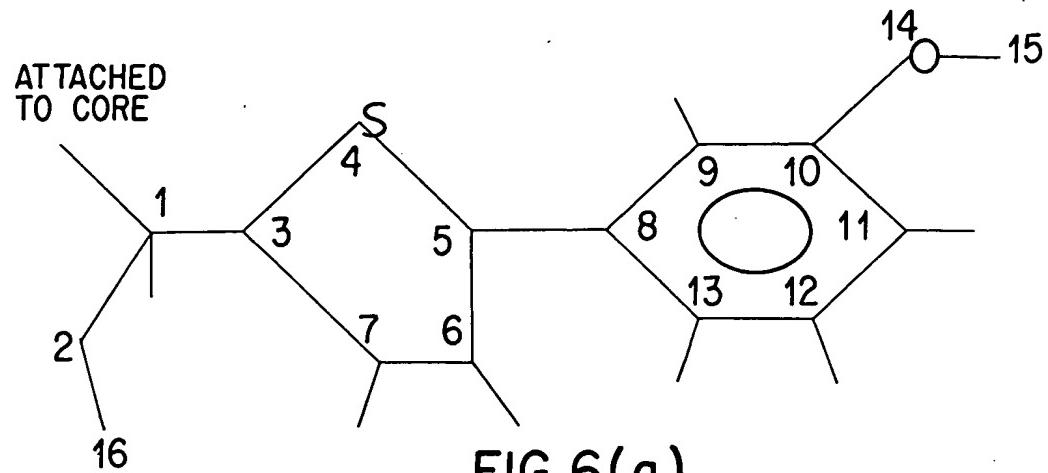


FIG. 5



0966543 - 0966544

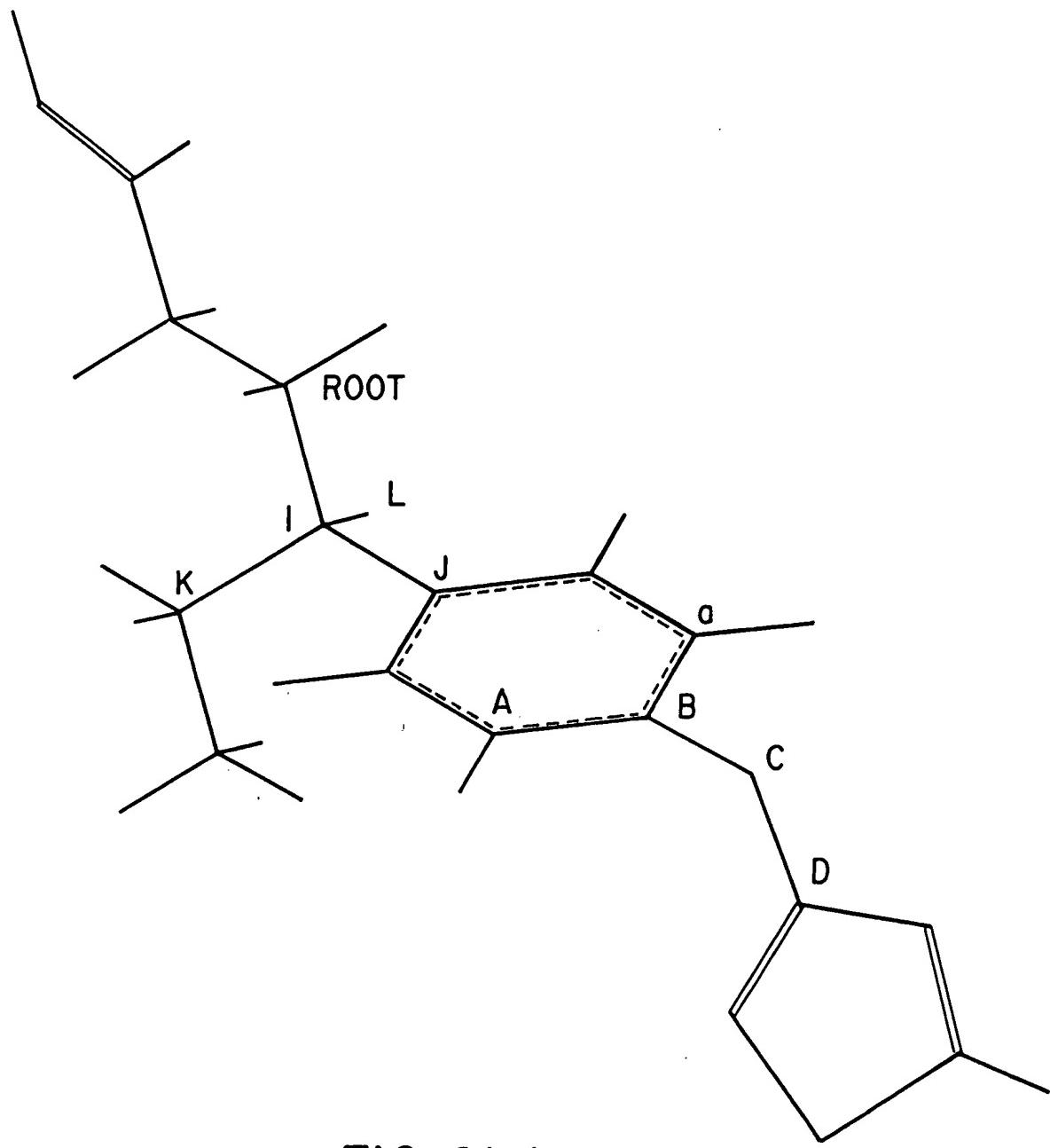


FIG. 6(d)

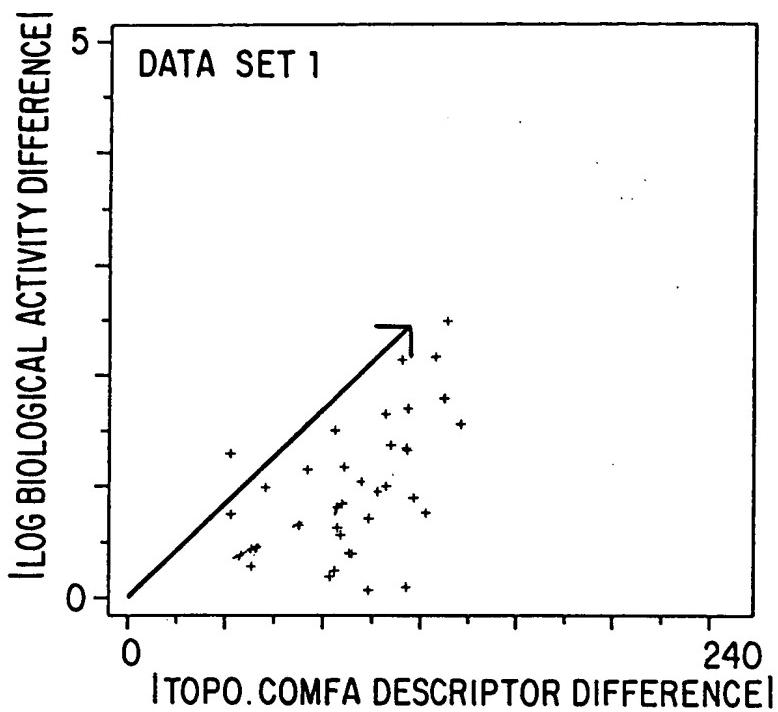


FIG.7(a)

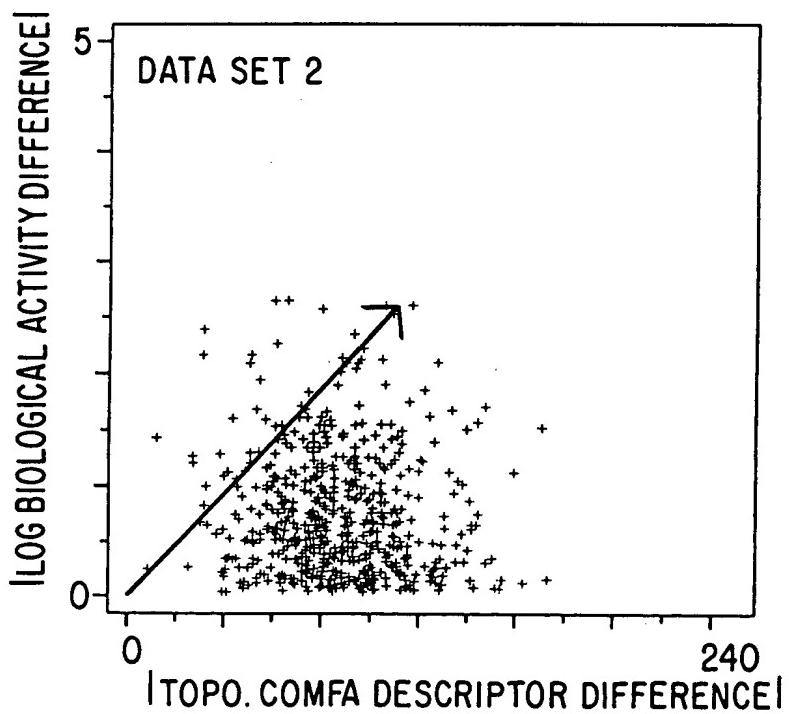


FIG.7(b)

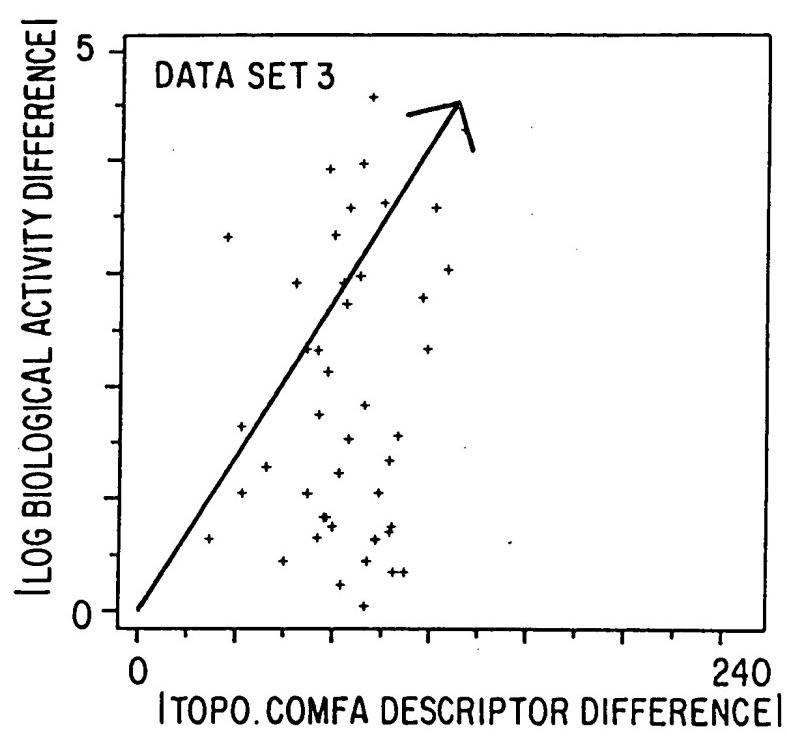


FIG.7(c)

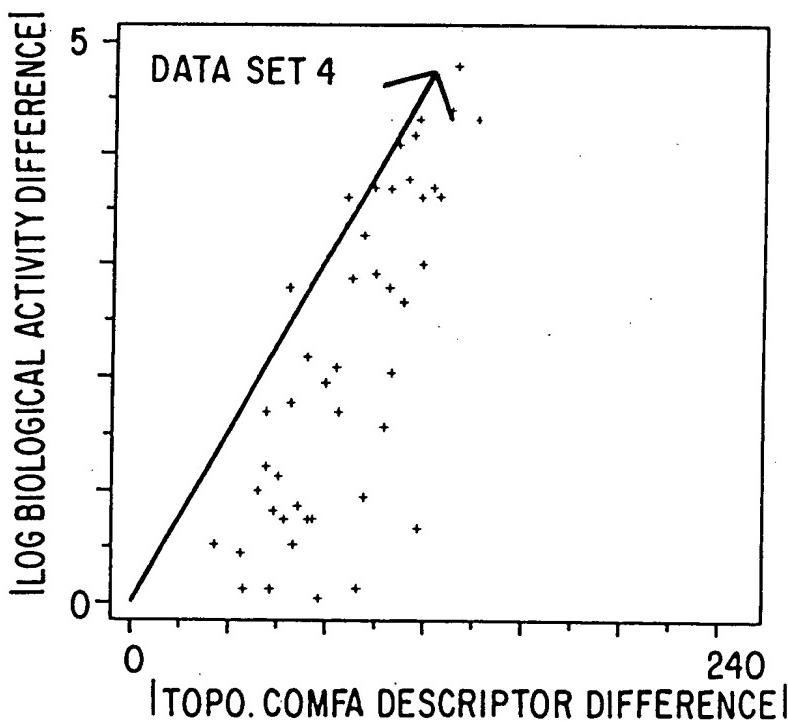


FIG.7(d)

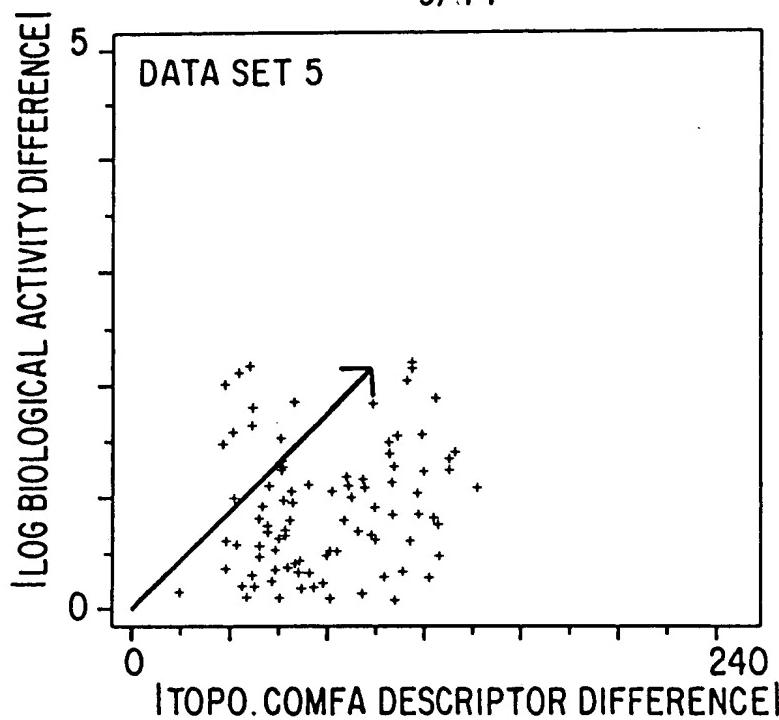


FIG.7(e)

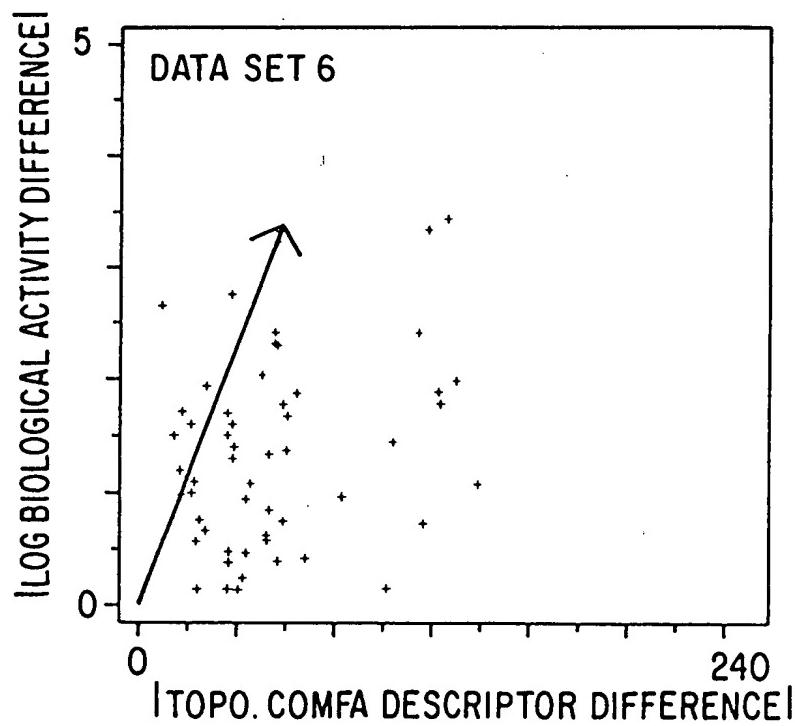


FIG.7(f)

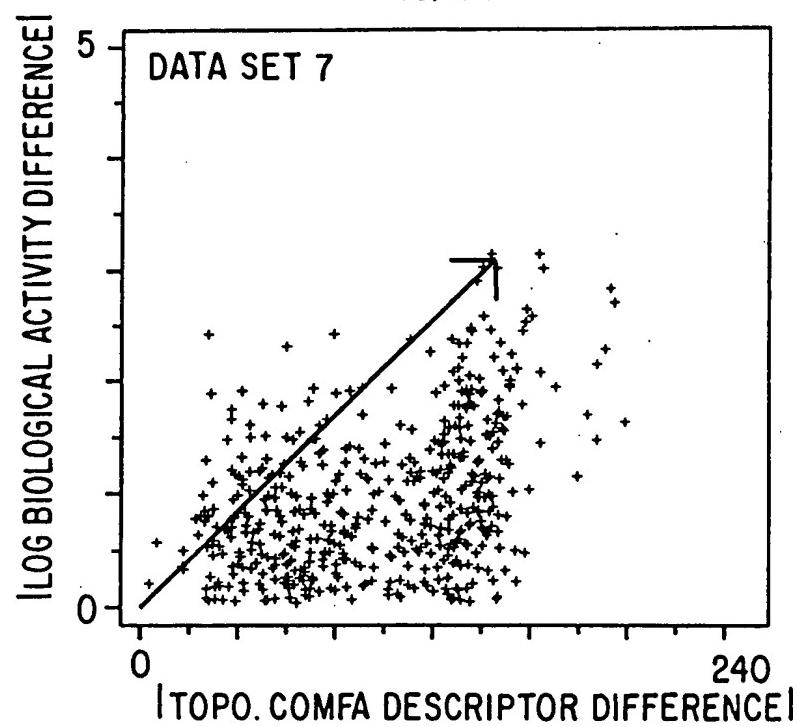


FIG.7(g)

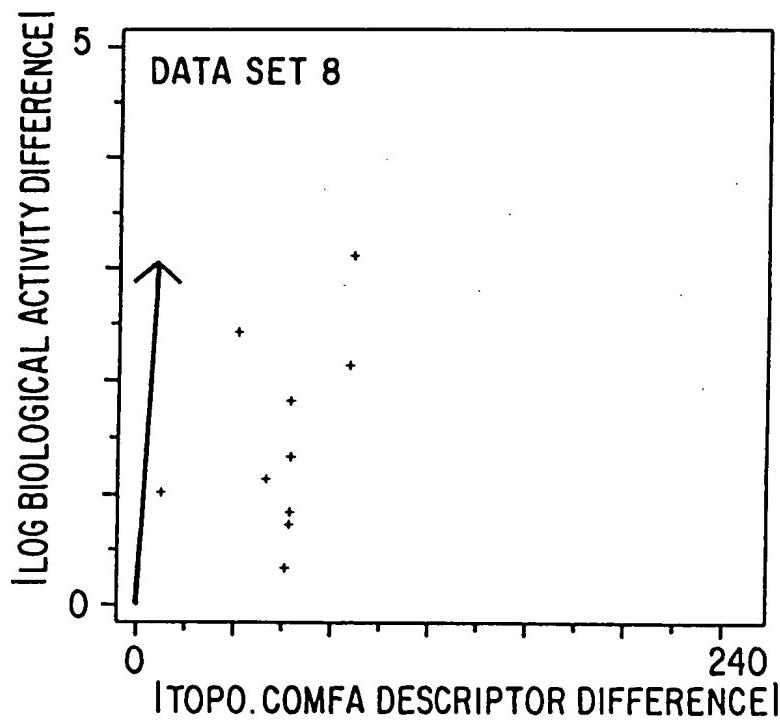


FIG.7(h)

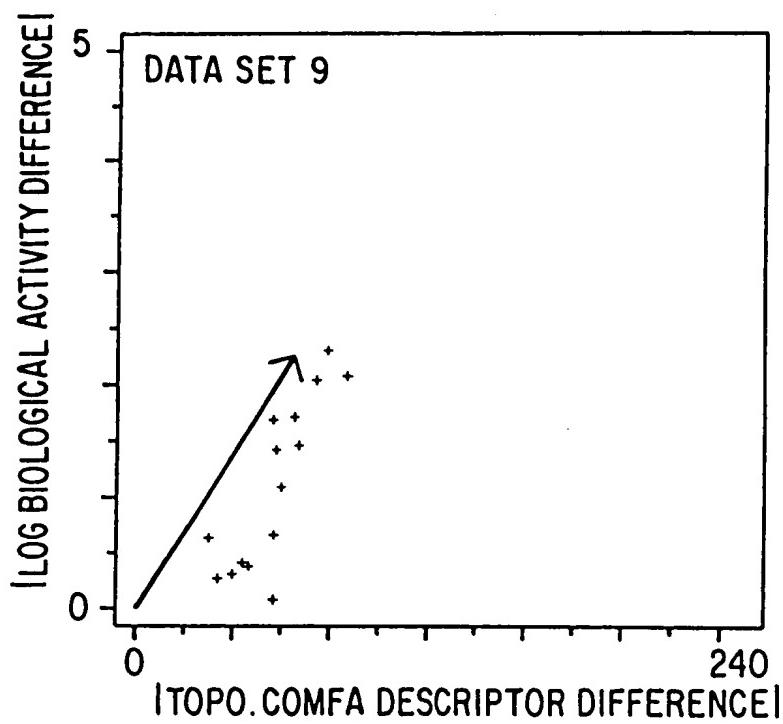


FIG.7(i)

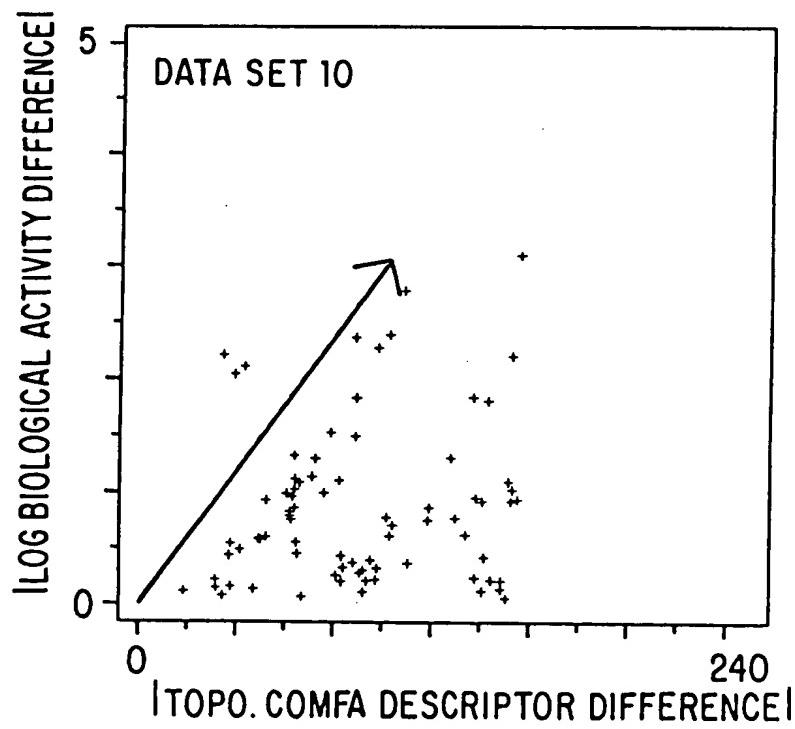


FIG.7(j)

T05250-E4599860

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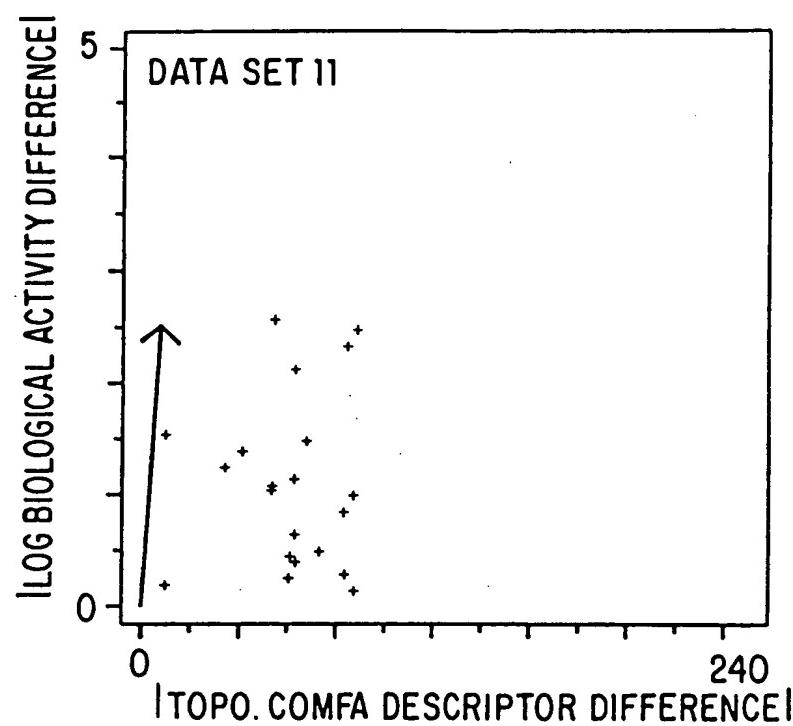


FIG.7(k)

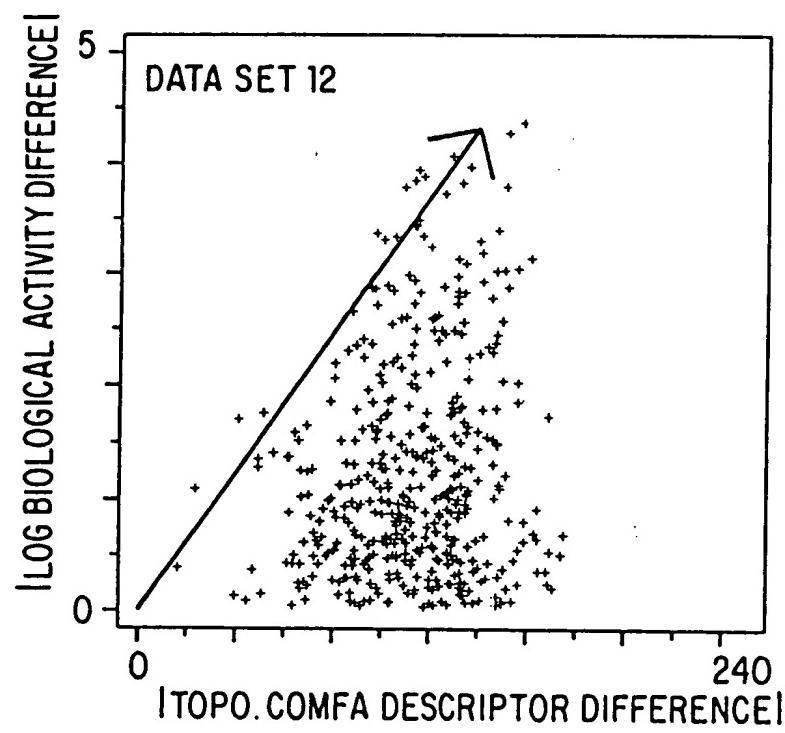


FIG.7(l)

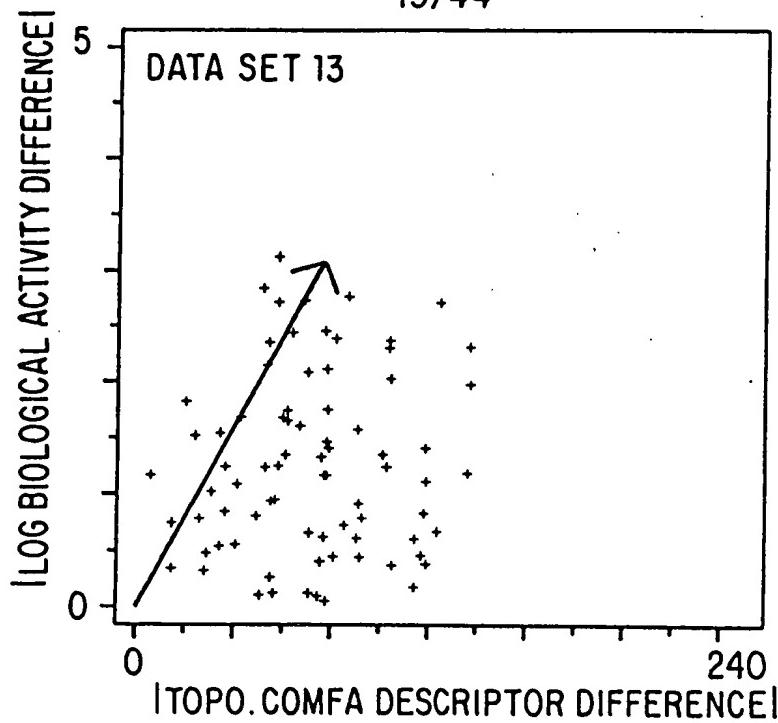


FIG.7(m)

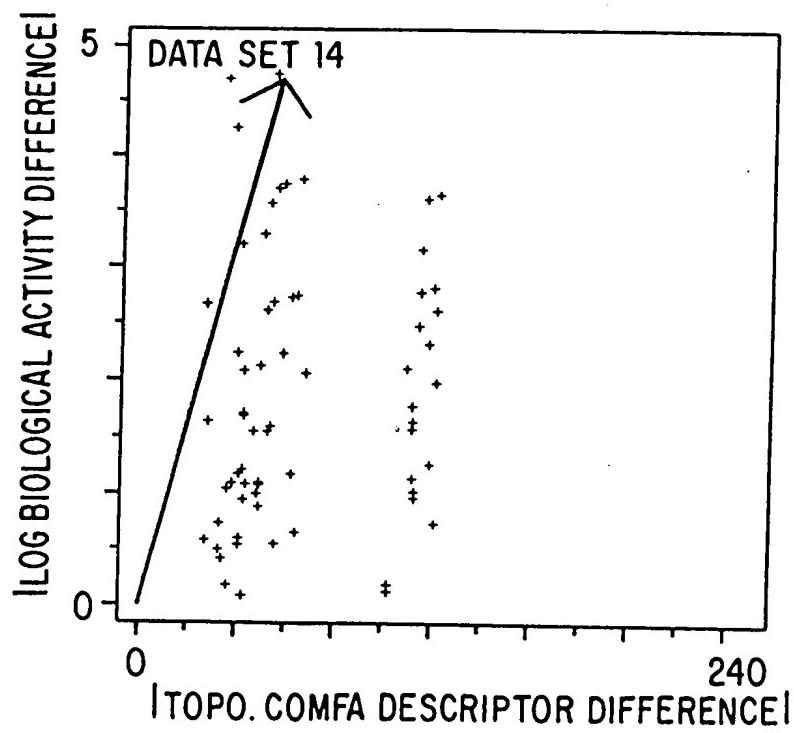


FIG.7(n)

F05250 "E415999860

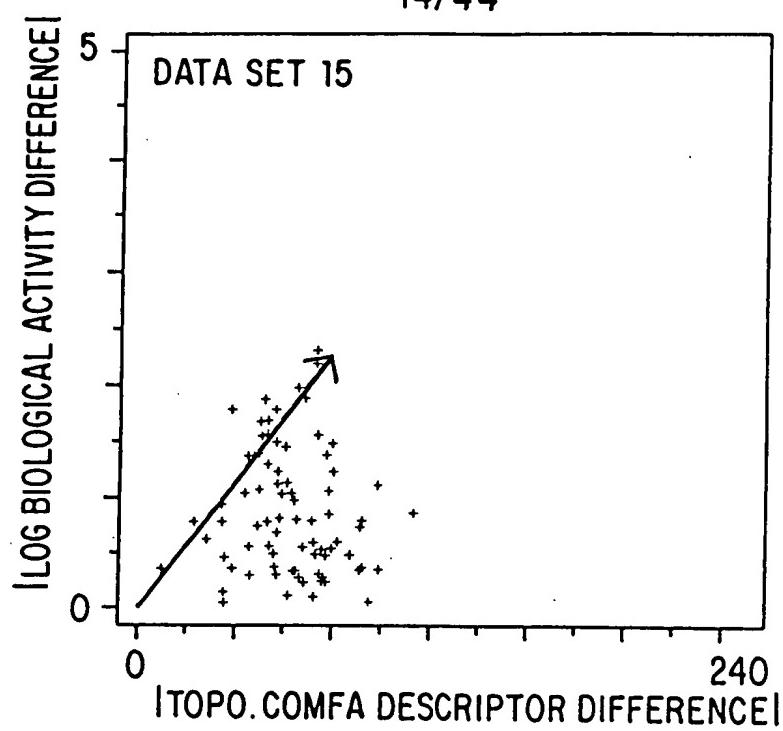


FIG.7(o)

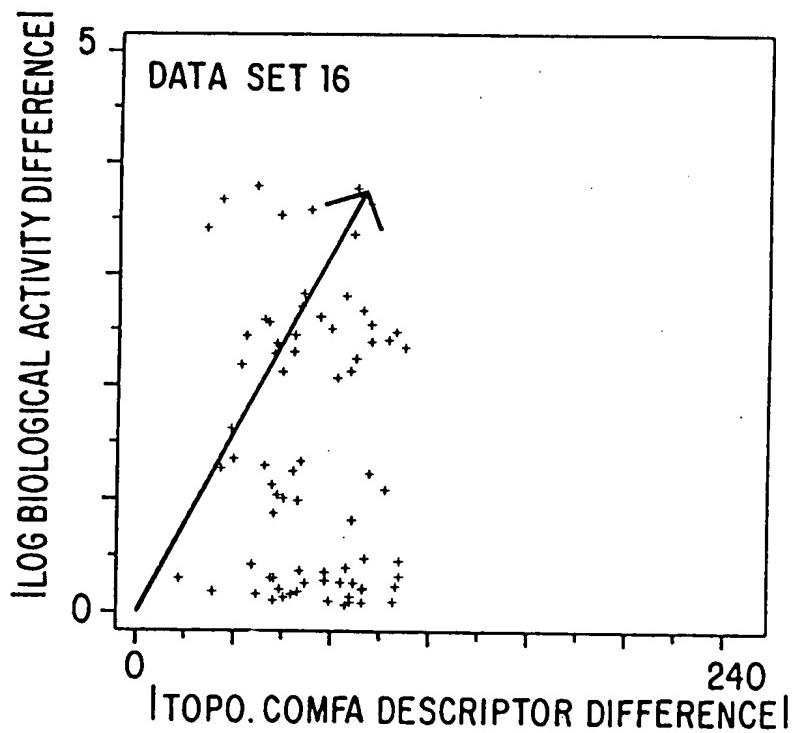


FIG.7(p)

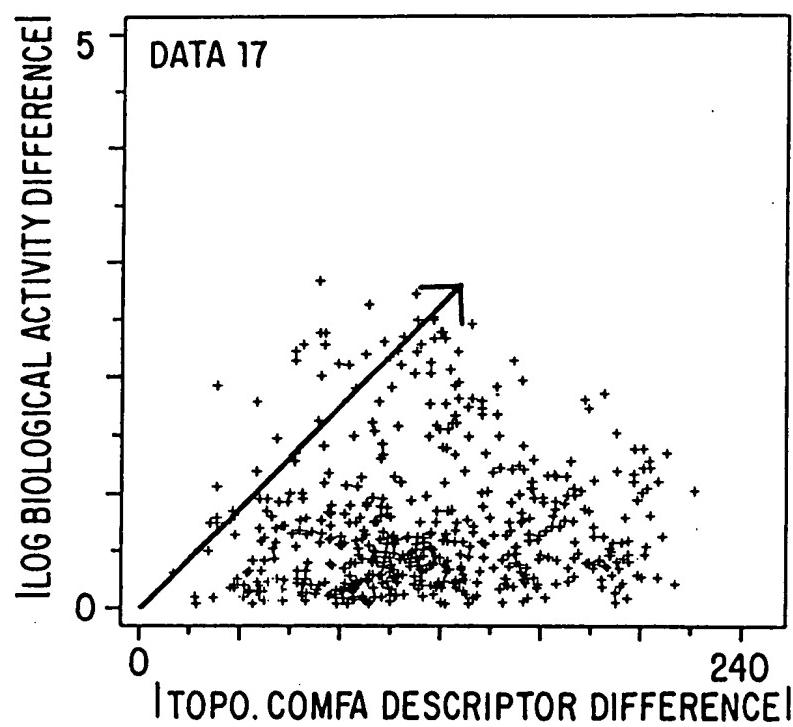


FIG. 7(q)

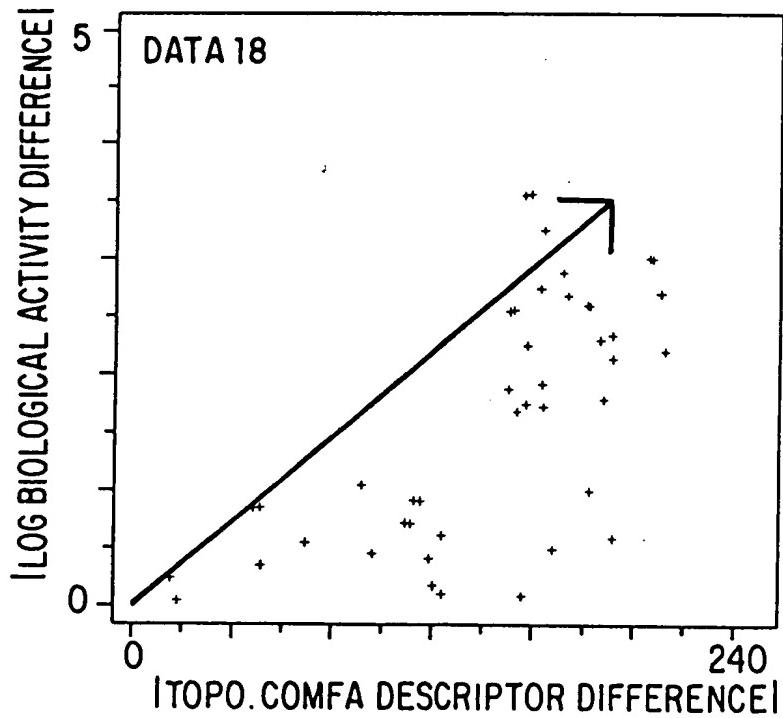
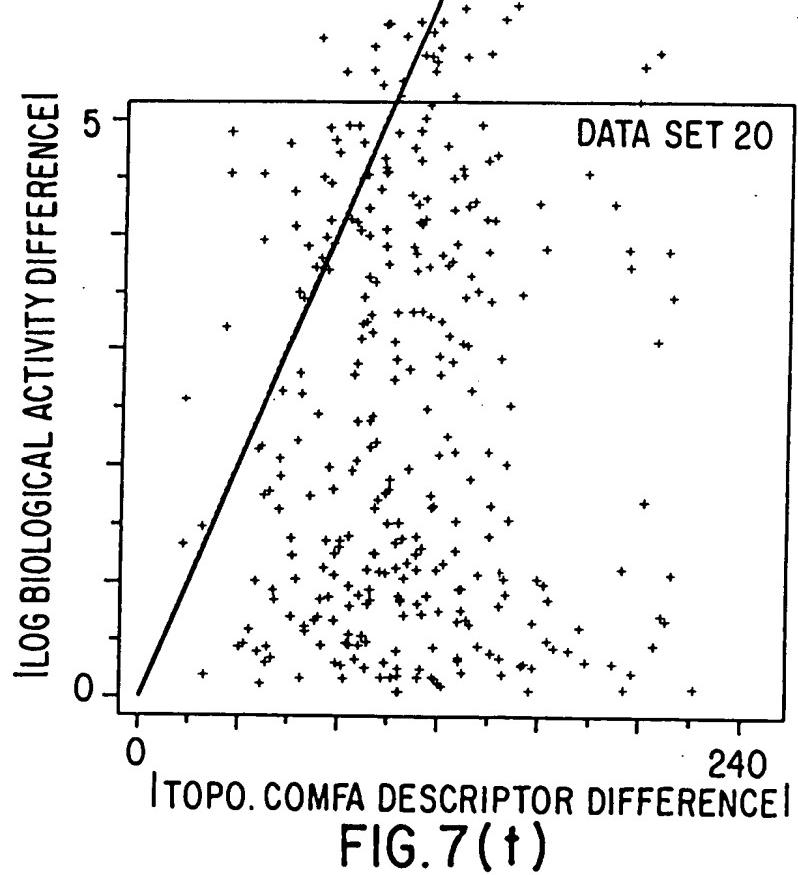
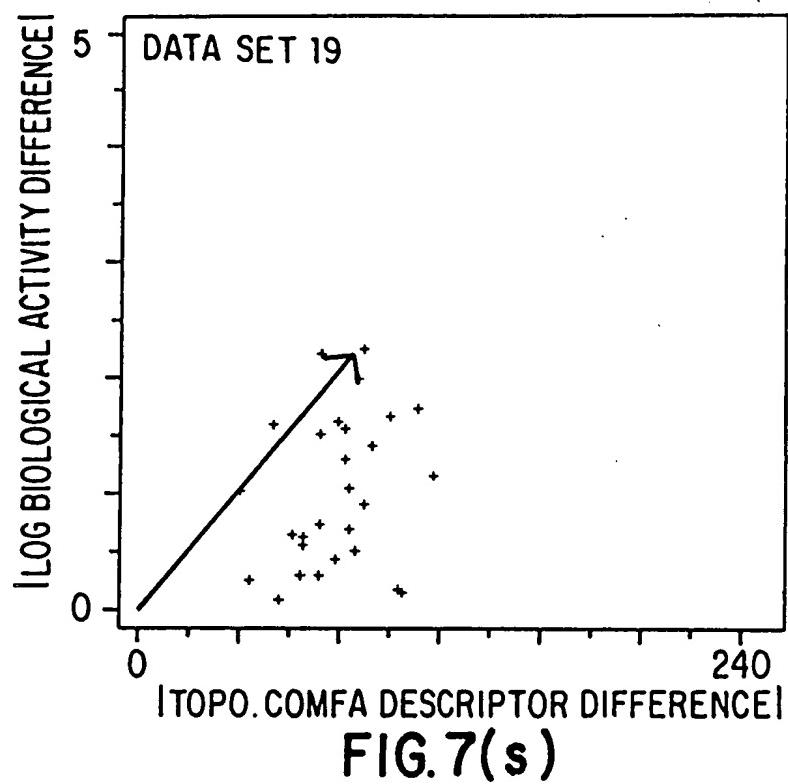


FIG. 7(r)

T05250 "E45998360



T05250 "E415599860

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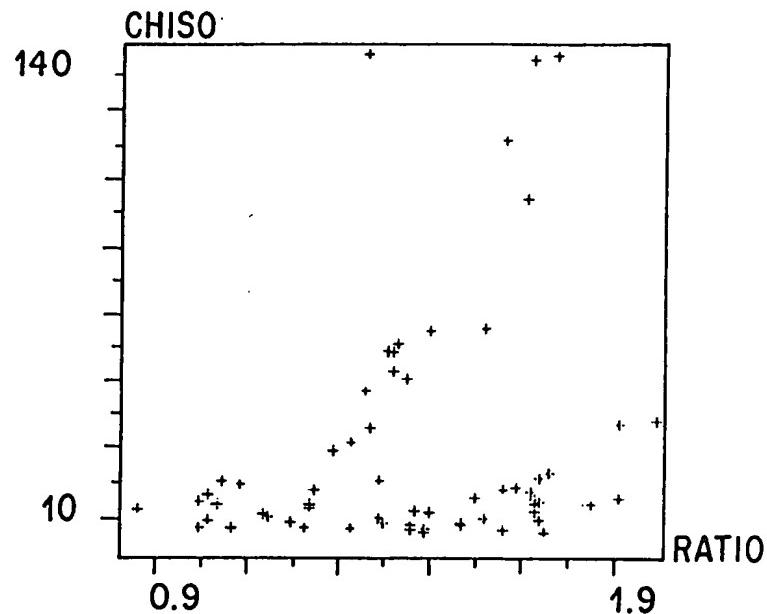


FIG. 8(a)

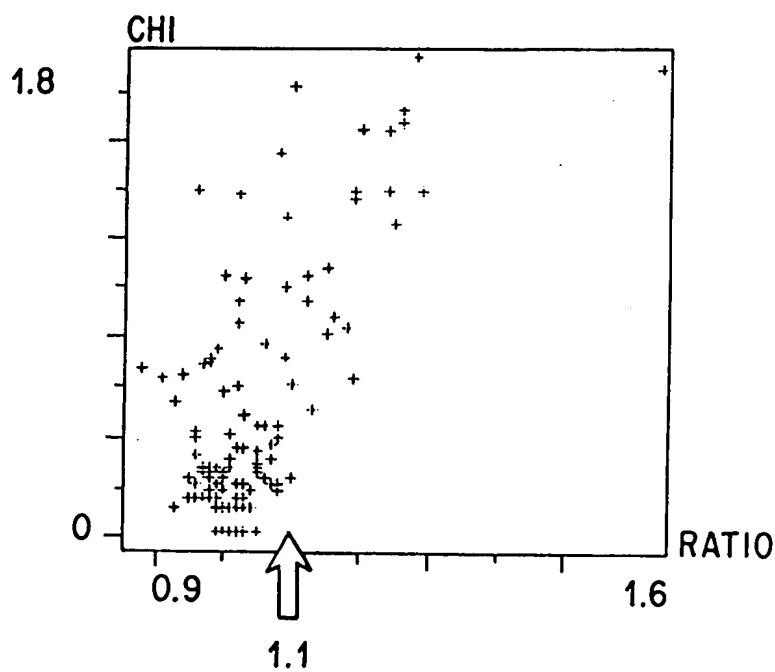


FIG. 8(b)

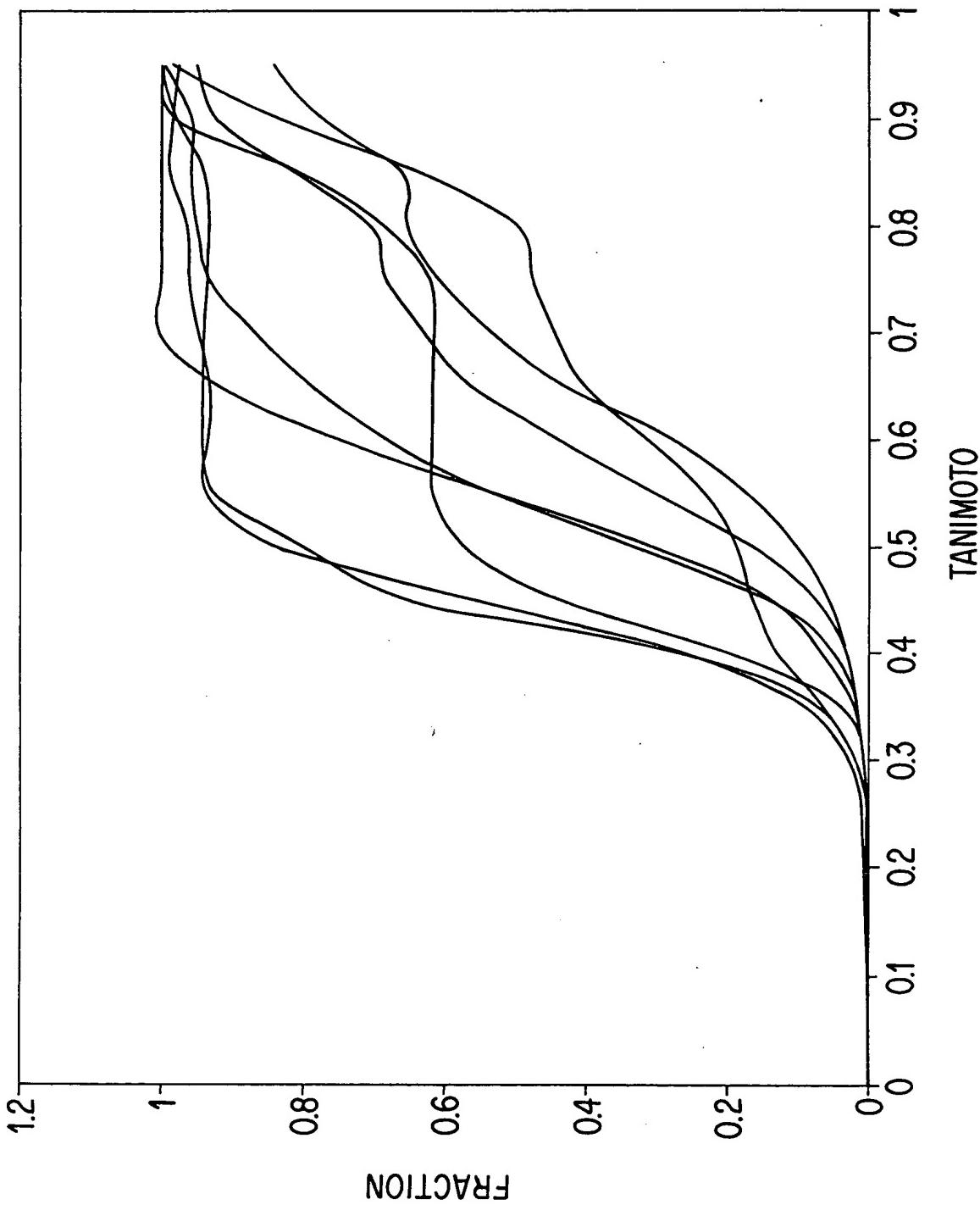


FIG. 9(a)

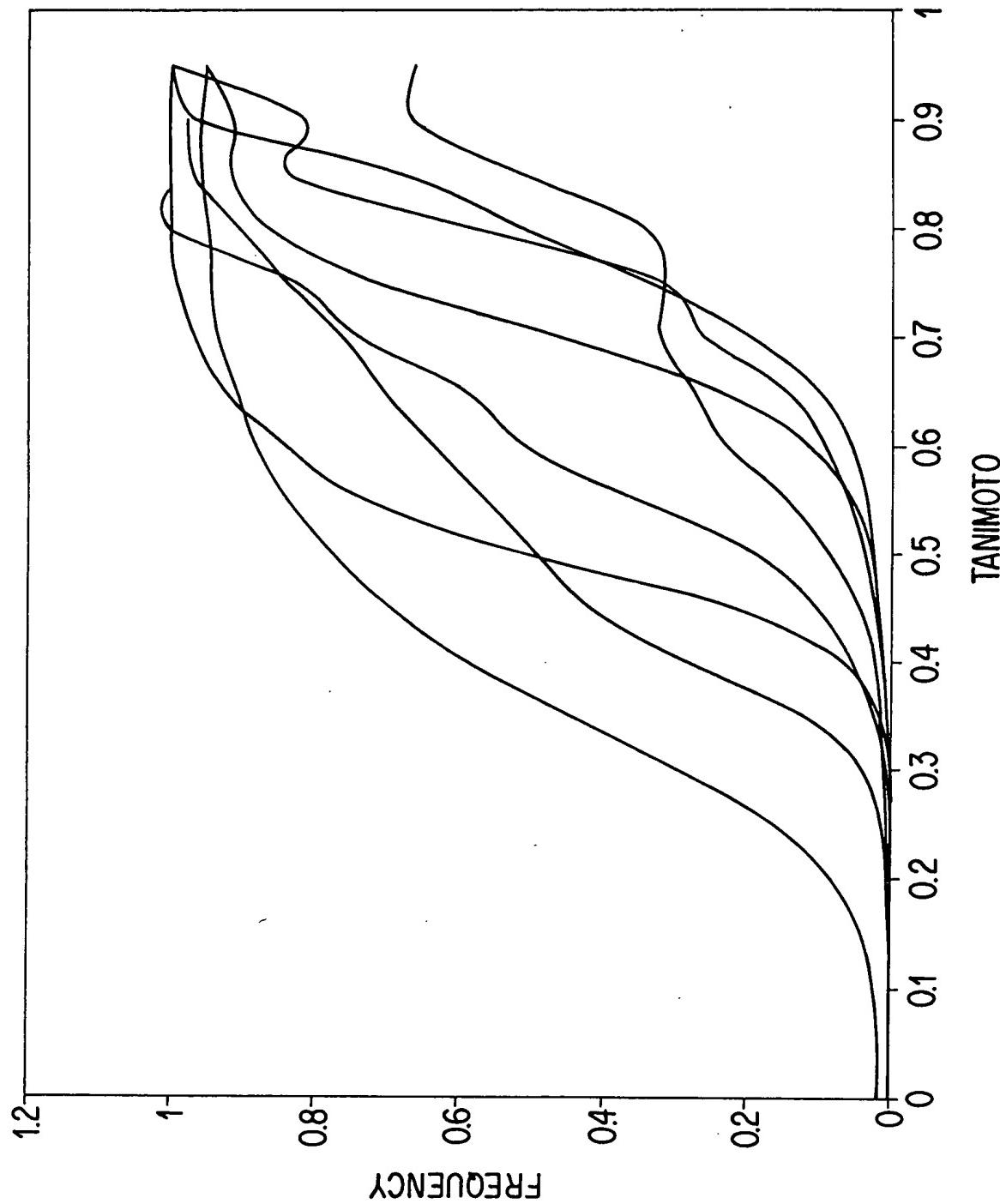
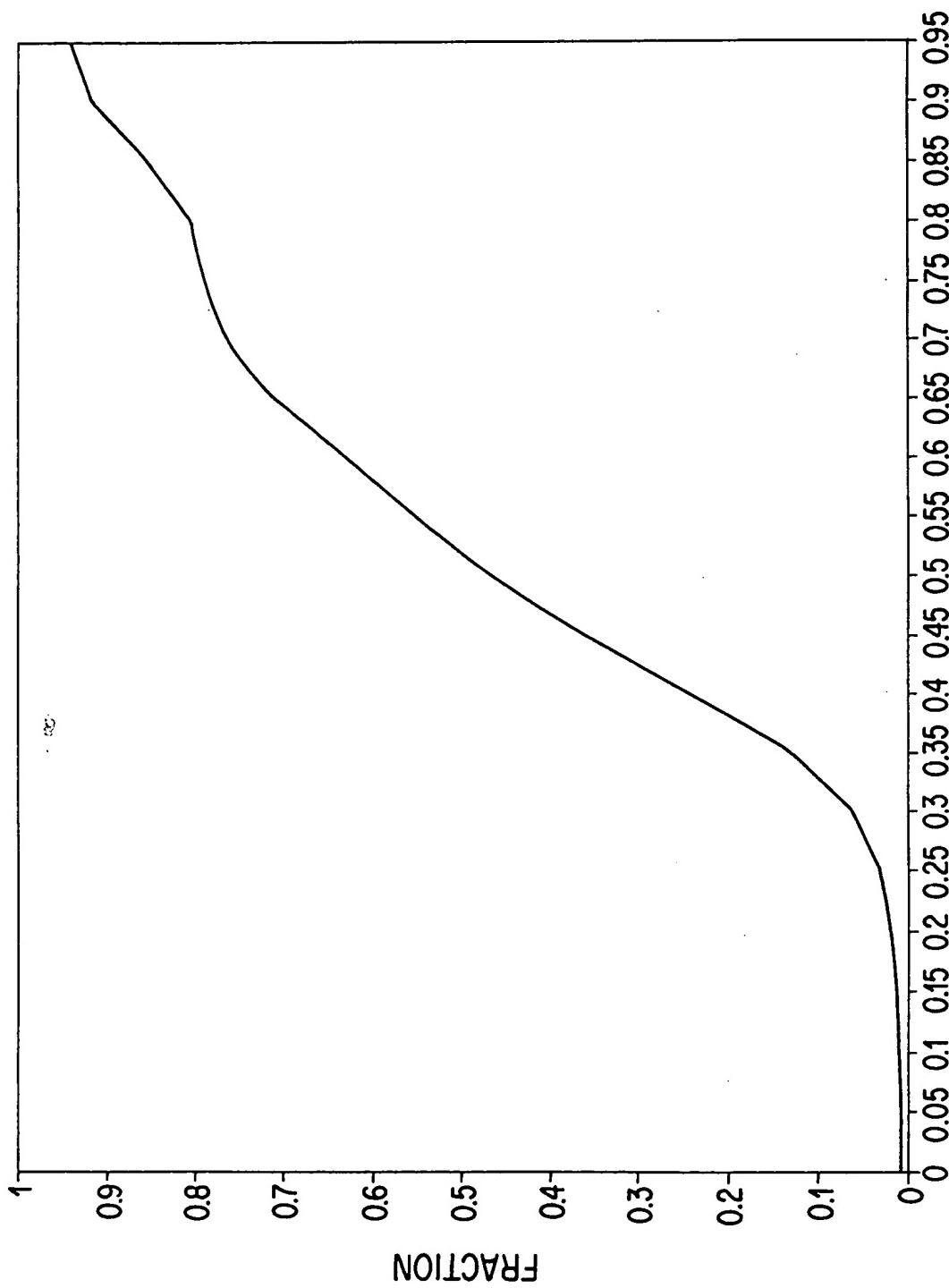


FIG. 9(b)



TANIMOTO

FIG. 9(c)

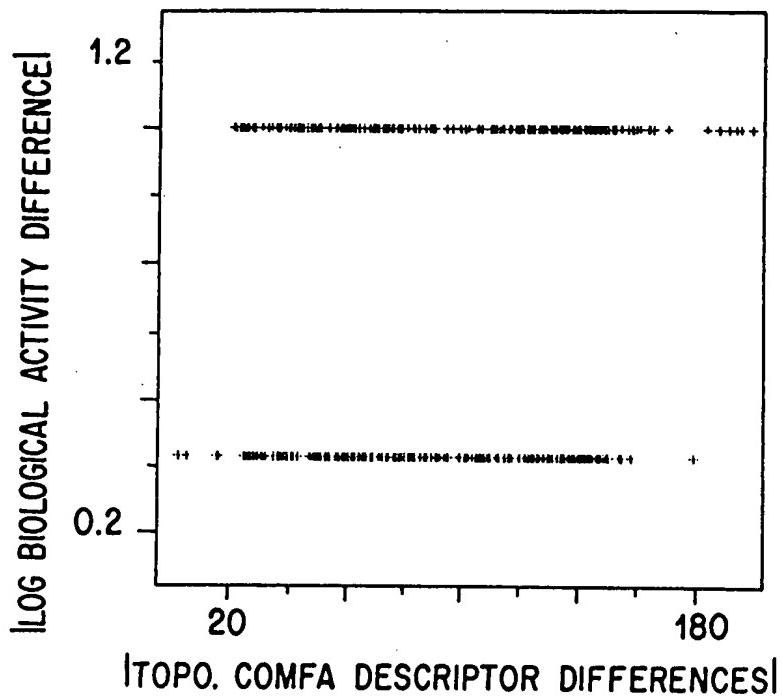


FIG.10(a)

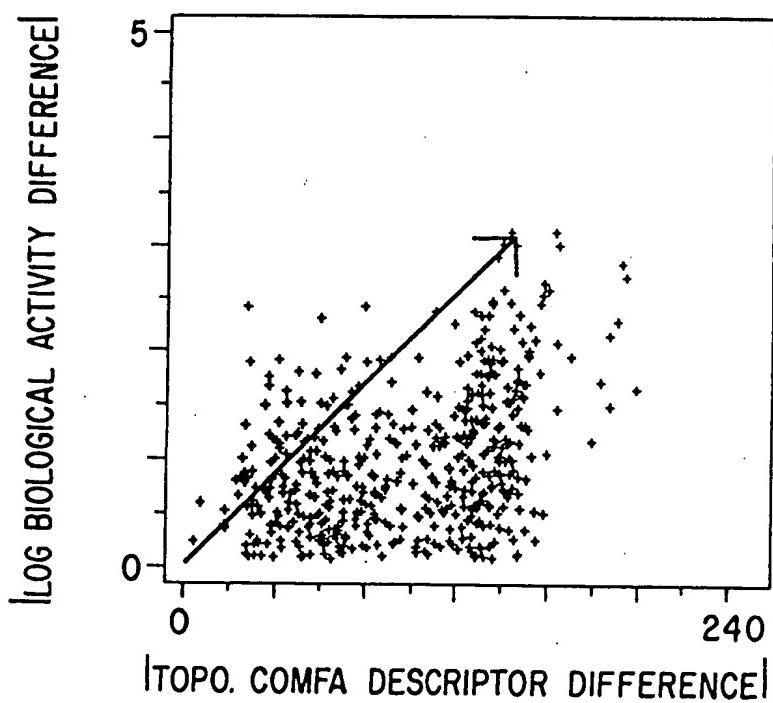


FIG.10(b)

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FUNCTION

8. A-
SELECT CHEMISTRY
LIST REACTANTS & CORES
DEFINE COMBINATIONS

8.A REMOVE REACTANTS: NON-DIVERSITY REASONS

8A(i) GENERAL CRITERIA
METALS
TAUTOMERS/SALTS & COUNT
INTERFERING GROUPS
SYNTHESIS & EXTRACTION
PRICE/AVAILABILITY

8.(A)ii BIOLOGICAL CRITERIA:
TOXIC/METABOLICALLY
HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP
NON-BILOGICALLY RELEVANT
GROUPS
SUGARS/MULTIPLE
FUNCTIONALITIES

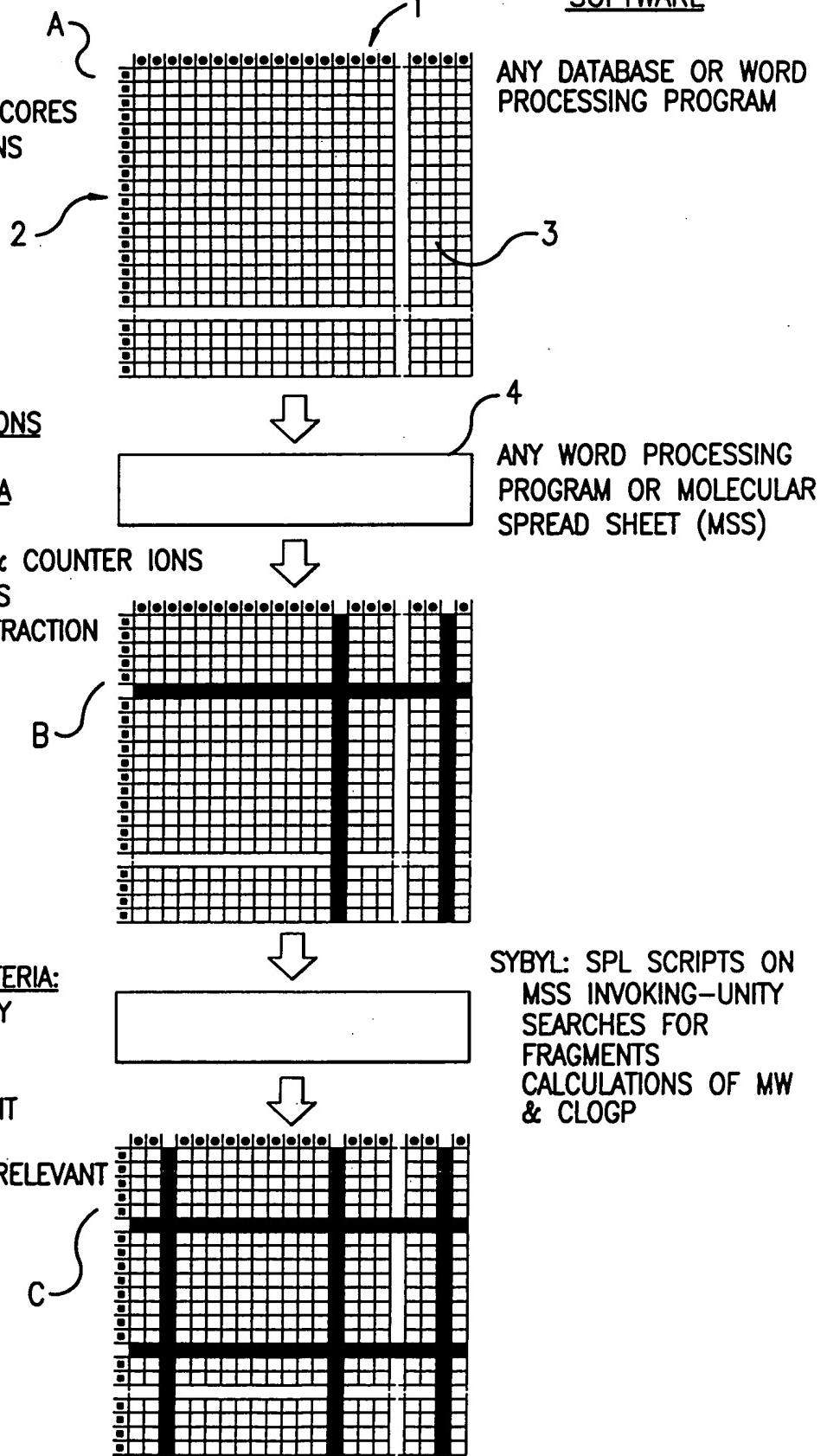


FIG.11(a)

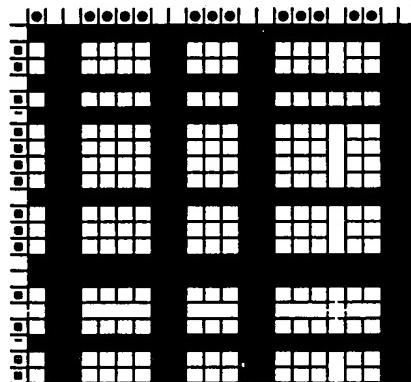
8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
TOPOMERIC CONFORMER
ALIGNMENT
CoMFA FIELD GENERATION:
HYDROGEN BOND FIELD
GENERATION
ROTATABLE BOND FIELD
ATTENUATION
CALCULATE FIELD
DIFFERENCES
CLUSTER
REACTANT SELECTION FROM
EACH CLUSTER

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SYBYL: SELECTOR &
CONCORD 3.2.1
SPECIALIZED SOFTWARE:
APPENDIX "A"
(SYBYL: CoMFA
STERIC & MSS)



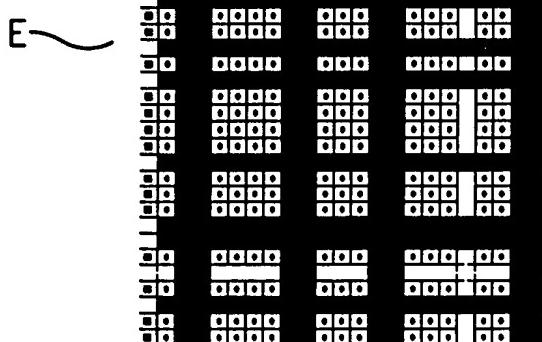
SYBYL: HIERCHICAL
CLUSTER - MSS
SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS



SYBYL: LEGION MSS



8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:



SYBYL: SPL SCRIPTS
ON MSS

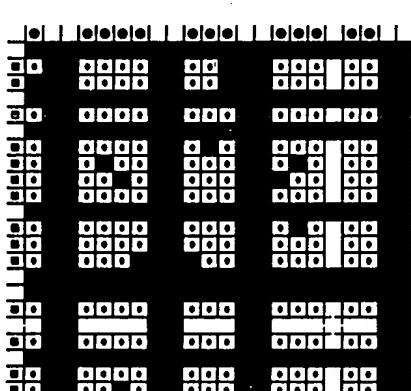


FIG.11(b)

8D

BIOLOGICAL CRITERIA:

METABOLICALLY HAZARDOUS

BIOAVAILABILITY

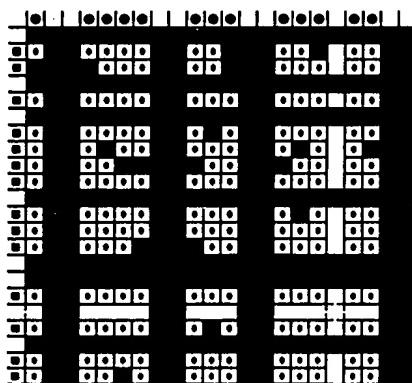
MOLECULAR WEIGHT

CLOGP

G



SYBYL: SPL SCRIPTS ON
MSS INVOKING –
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP



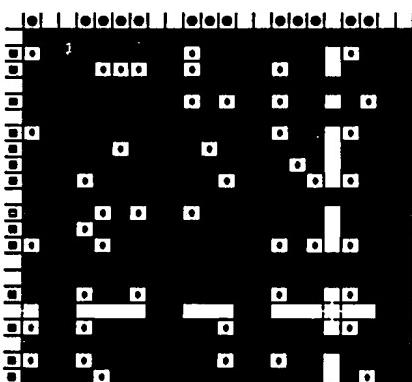
8E

REMOVE NON-DIVERSE
PRODUCTS:GENERATE TANIMOTO
2D FINGERPRINTS

SAMPLE PRODUCTS:

EXCLUDE TAN \geq 0.85

UNITY

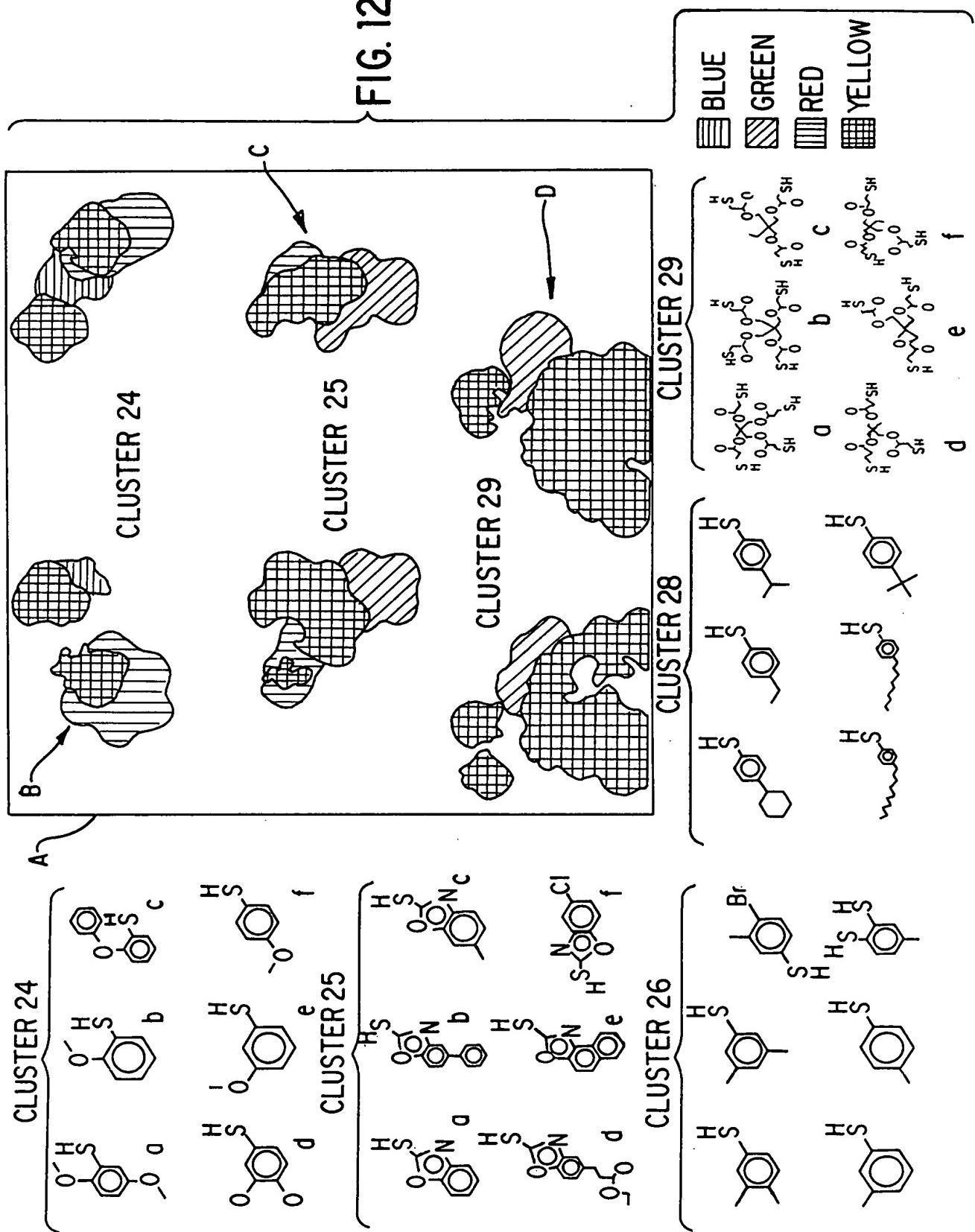


H

FIG.11(c)

09365143 - 052604

FIG. 12



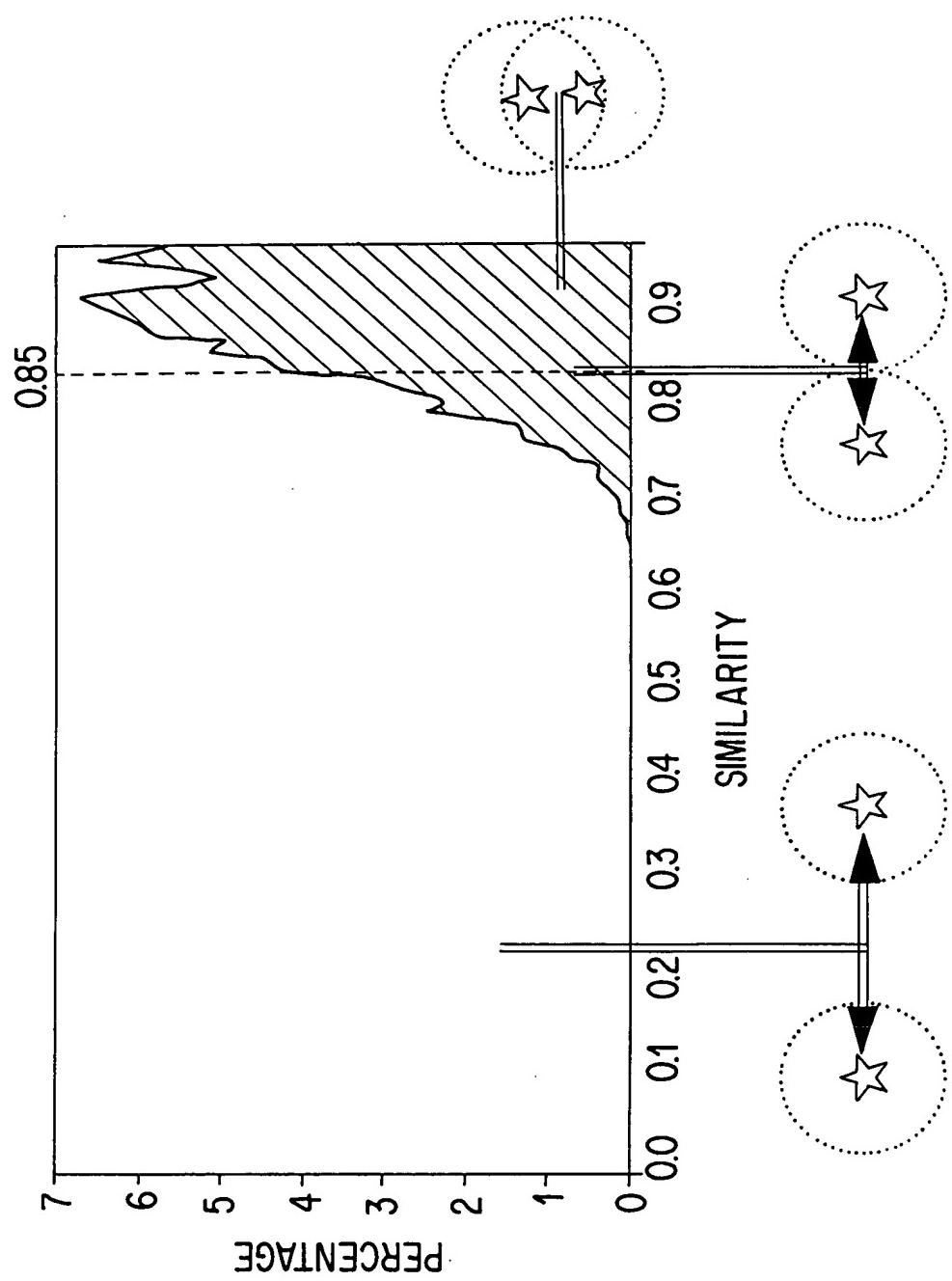


FIG. 13

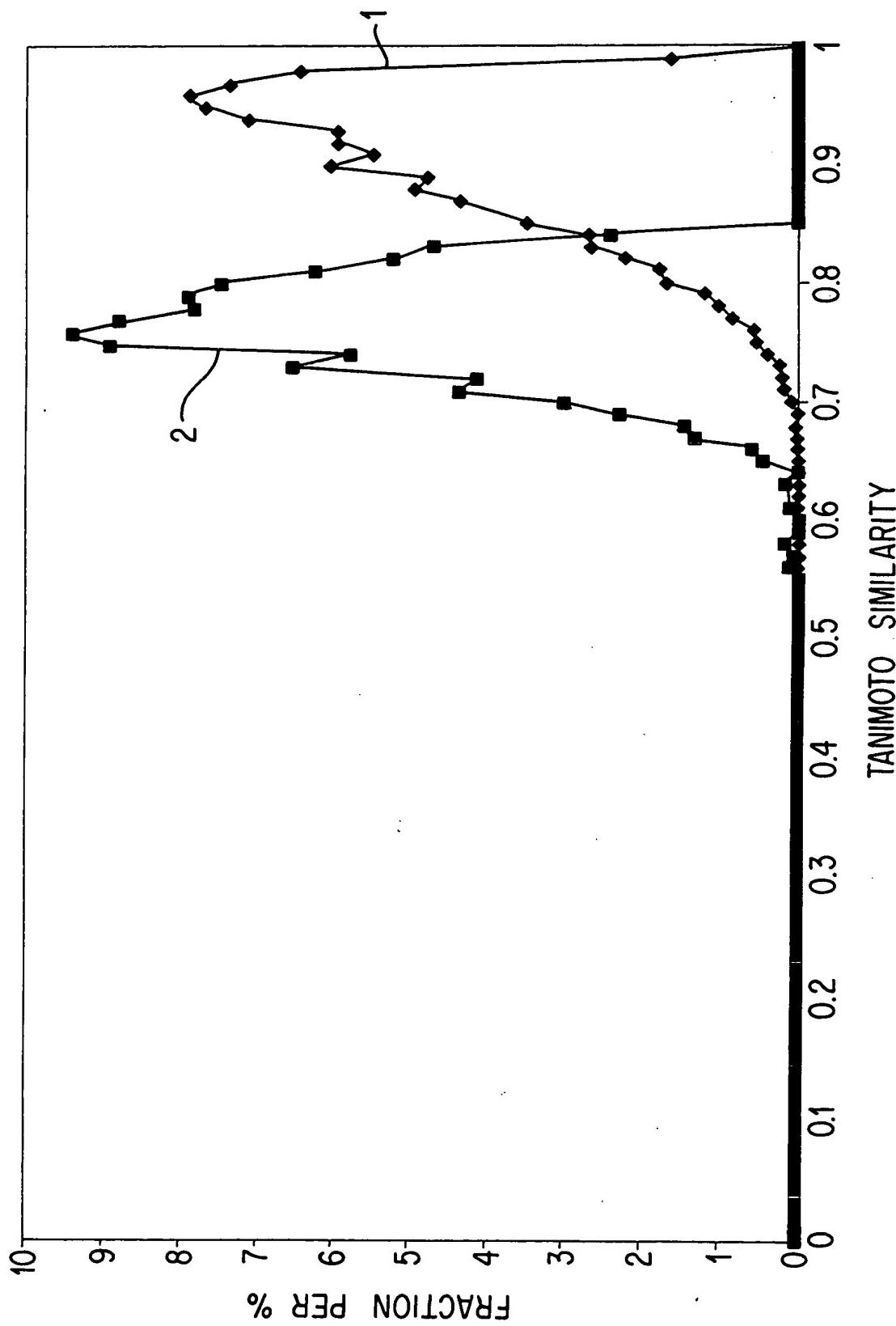
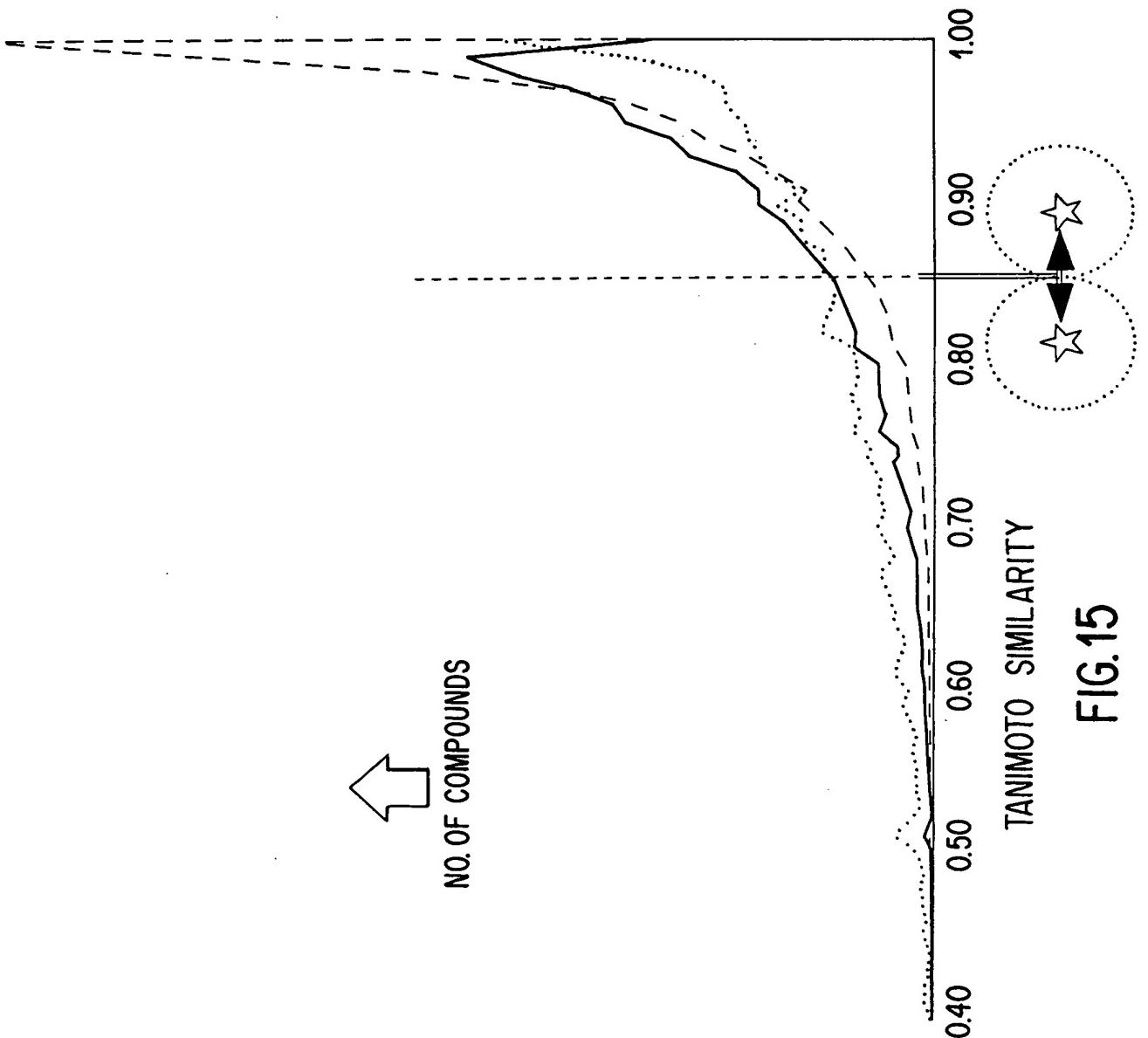


FIG. 14



卷之三

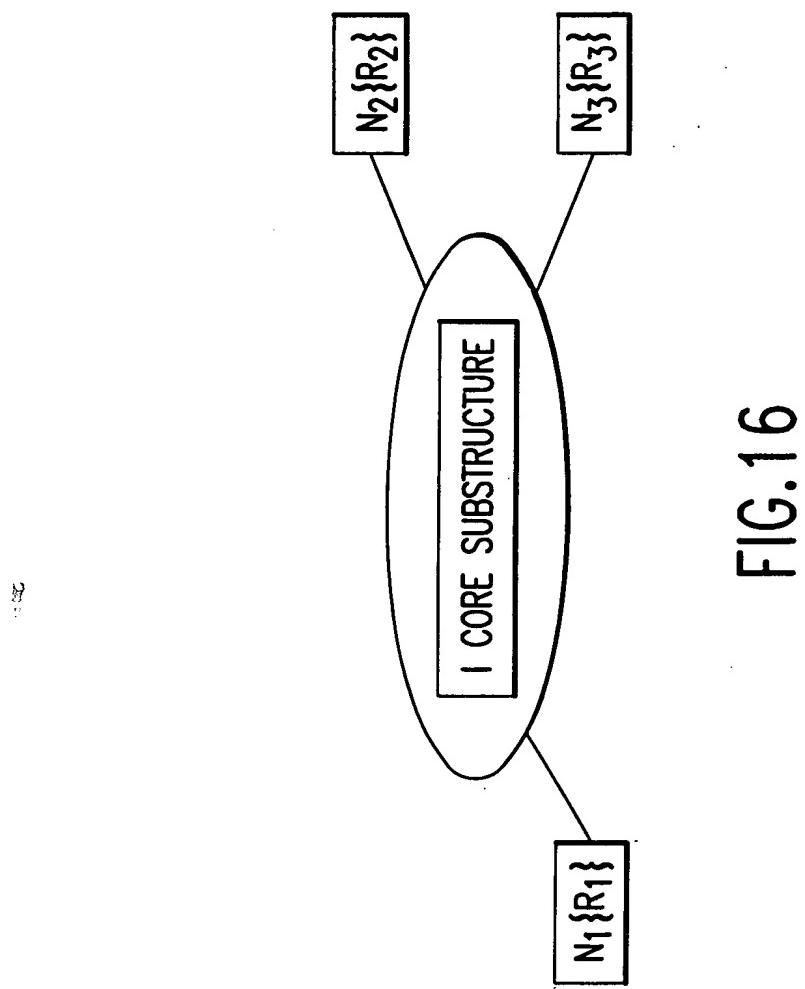


FIG. 16

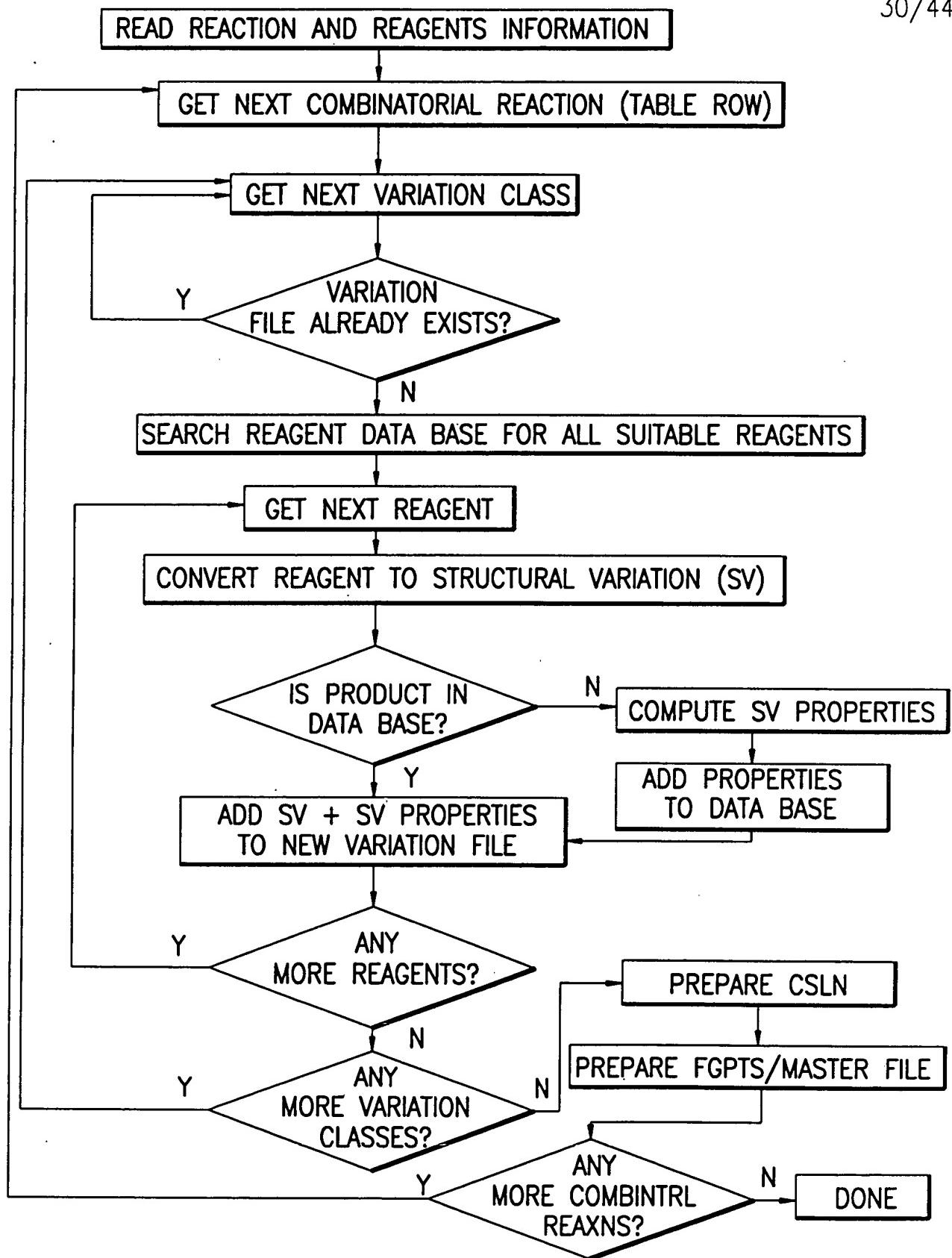


FIG.17

098655473 - 0525611

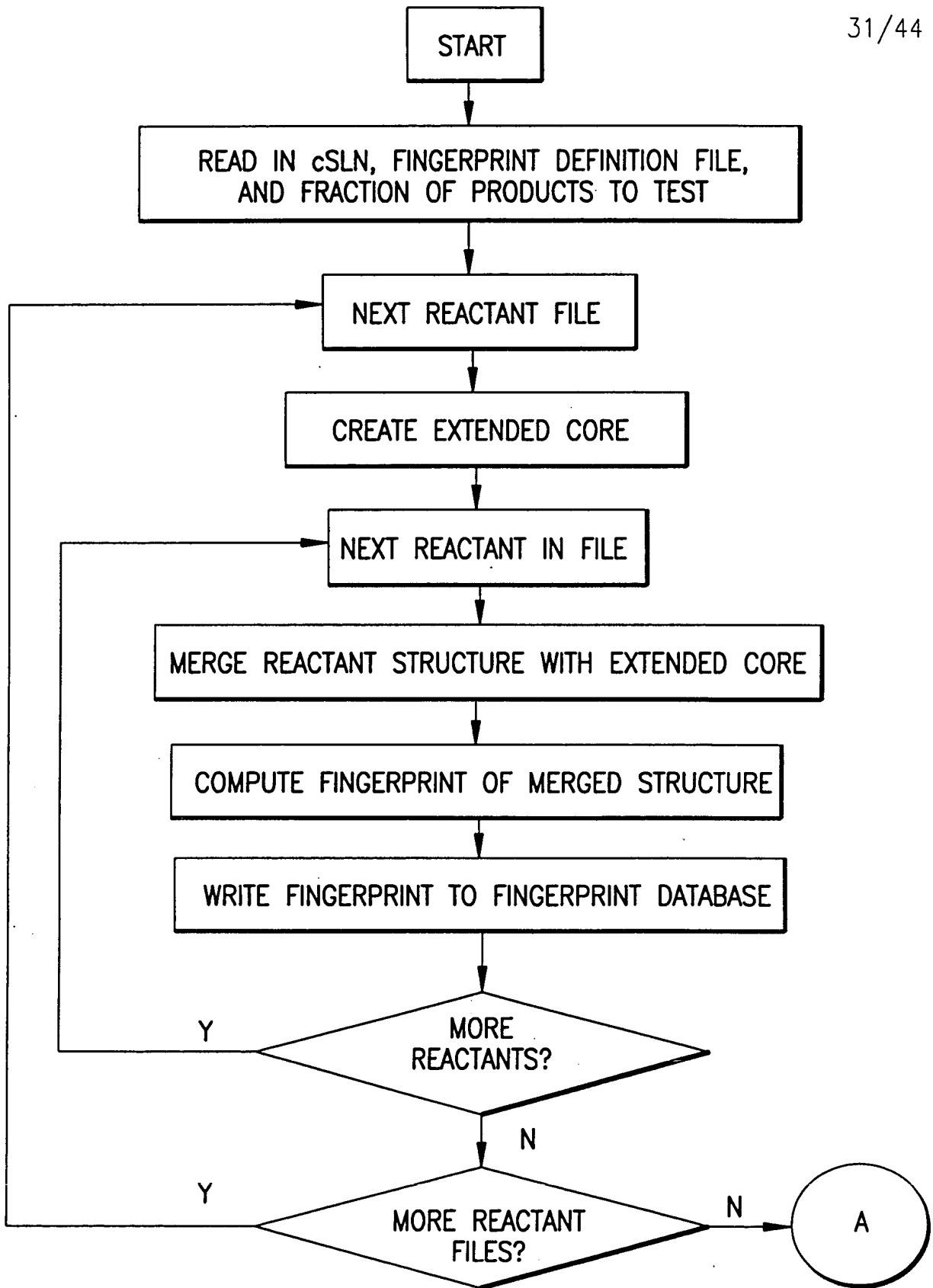


FIG.18

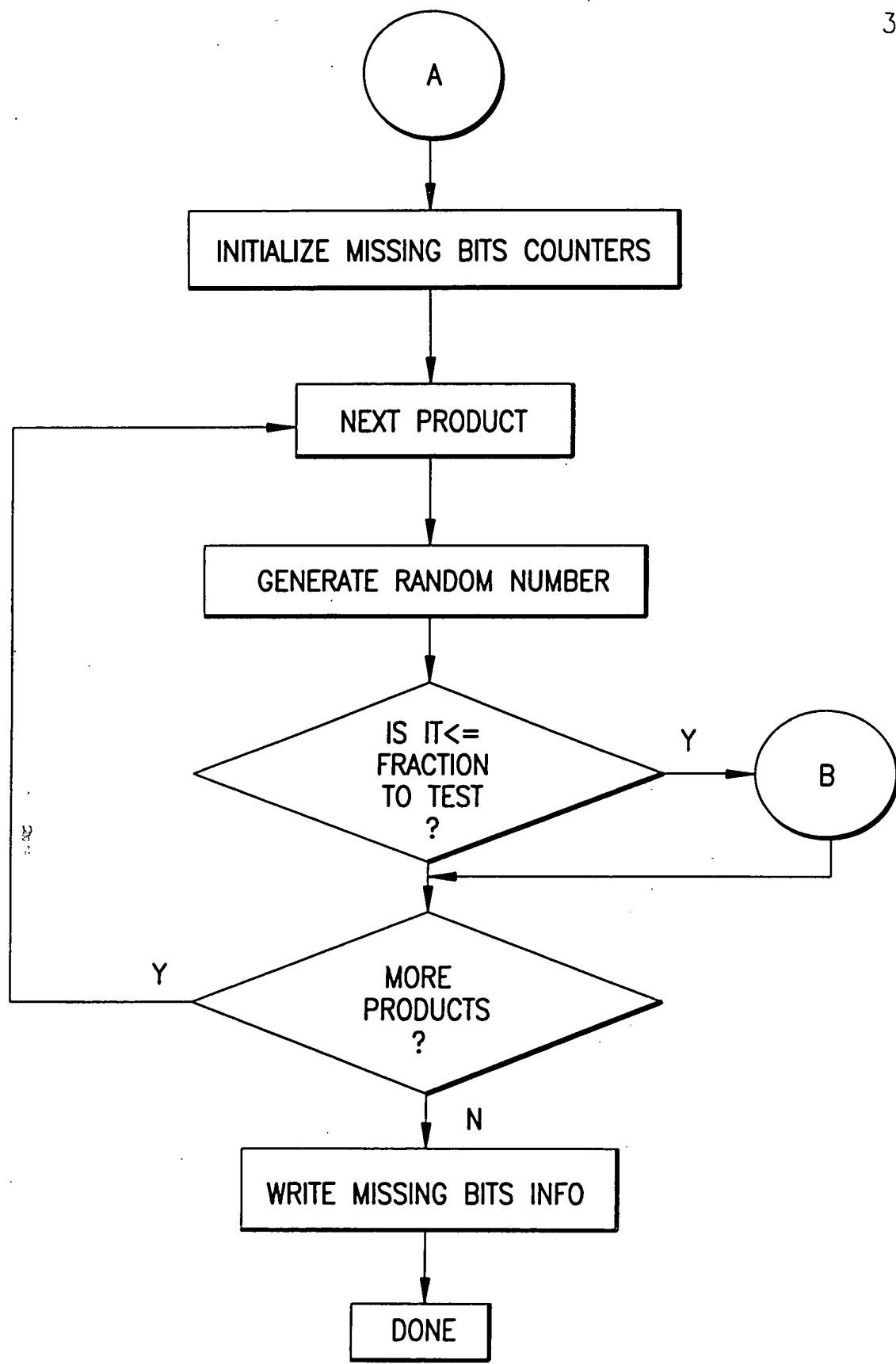


FIG.19

09366543 - 052501

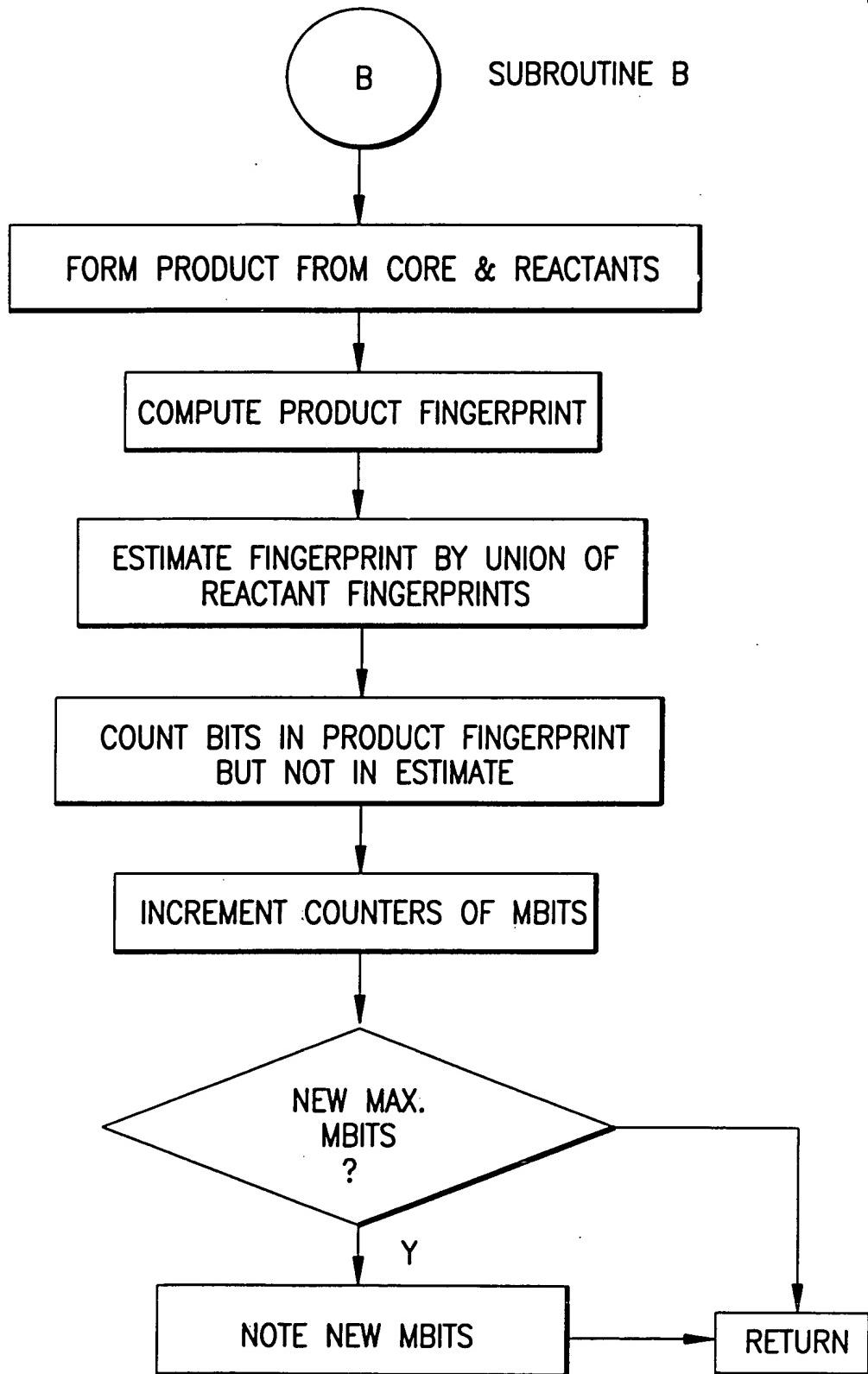


FIG.20

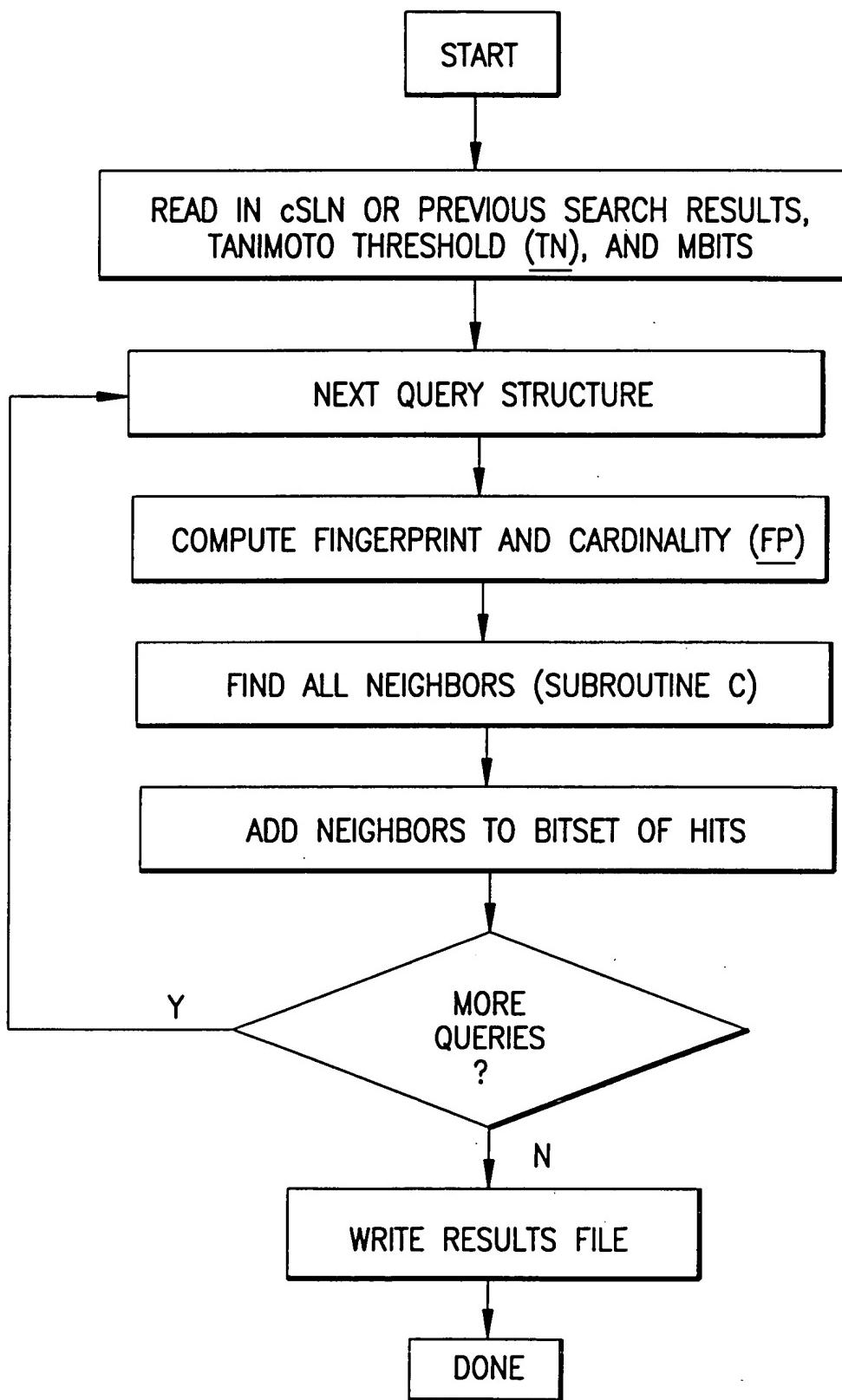


FIG.21

09666543 - 052504

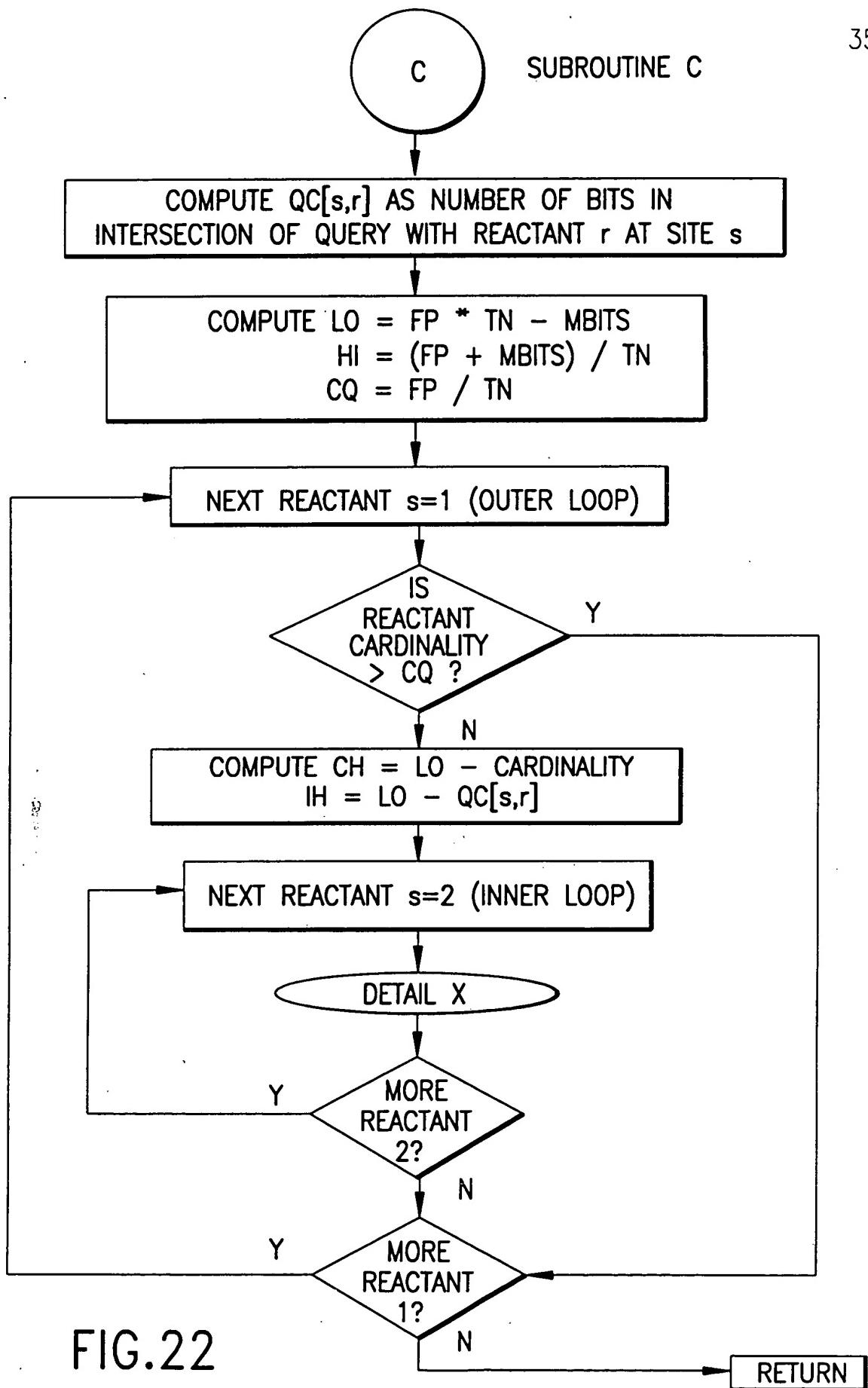


FIG.22

09366543-052501

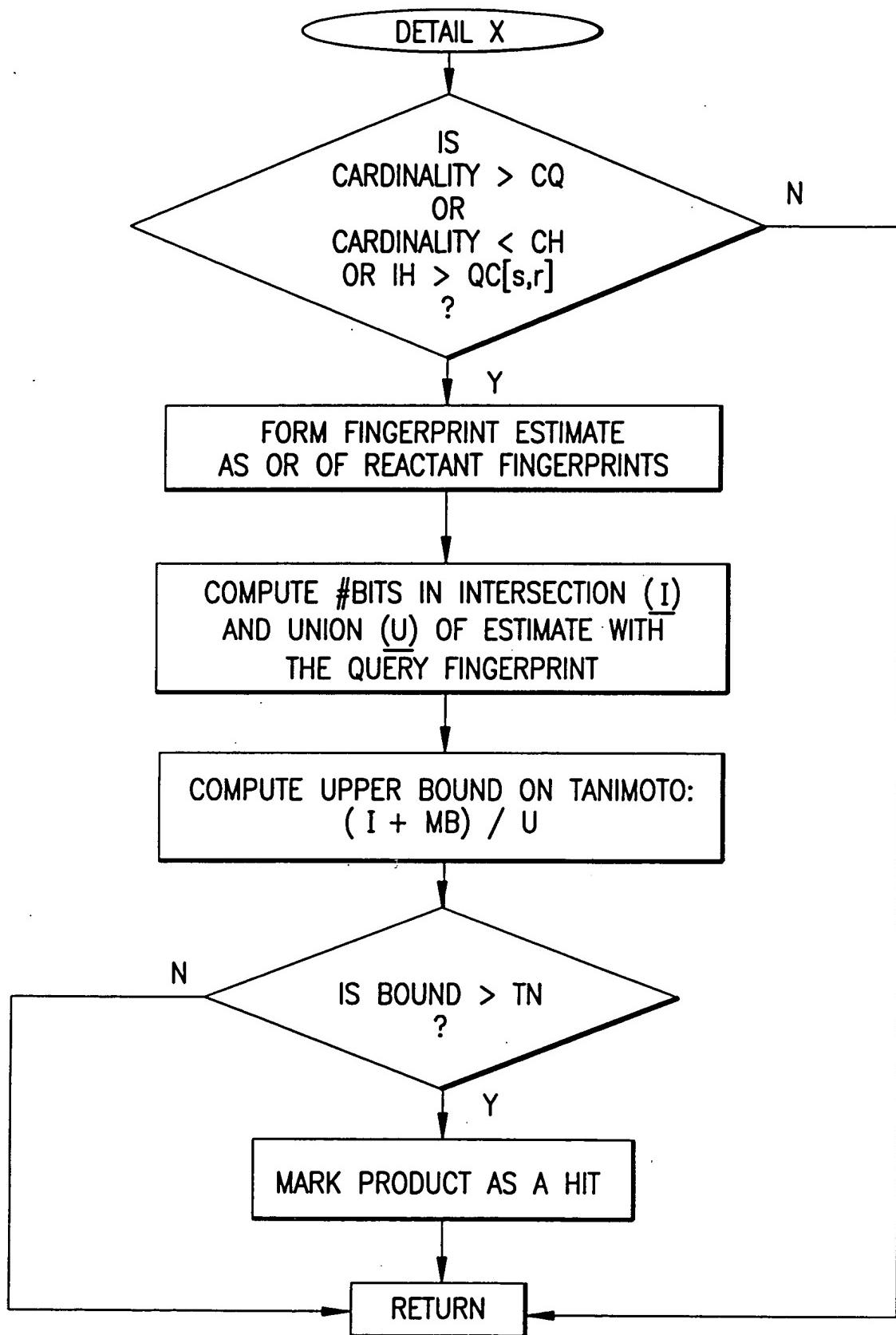


FIG.23

09366542 - 052504

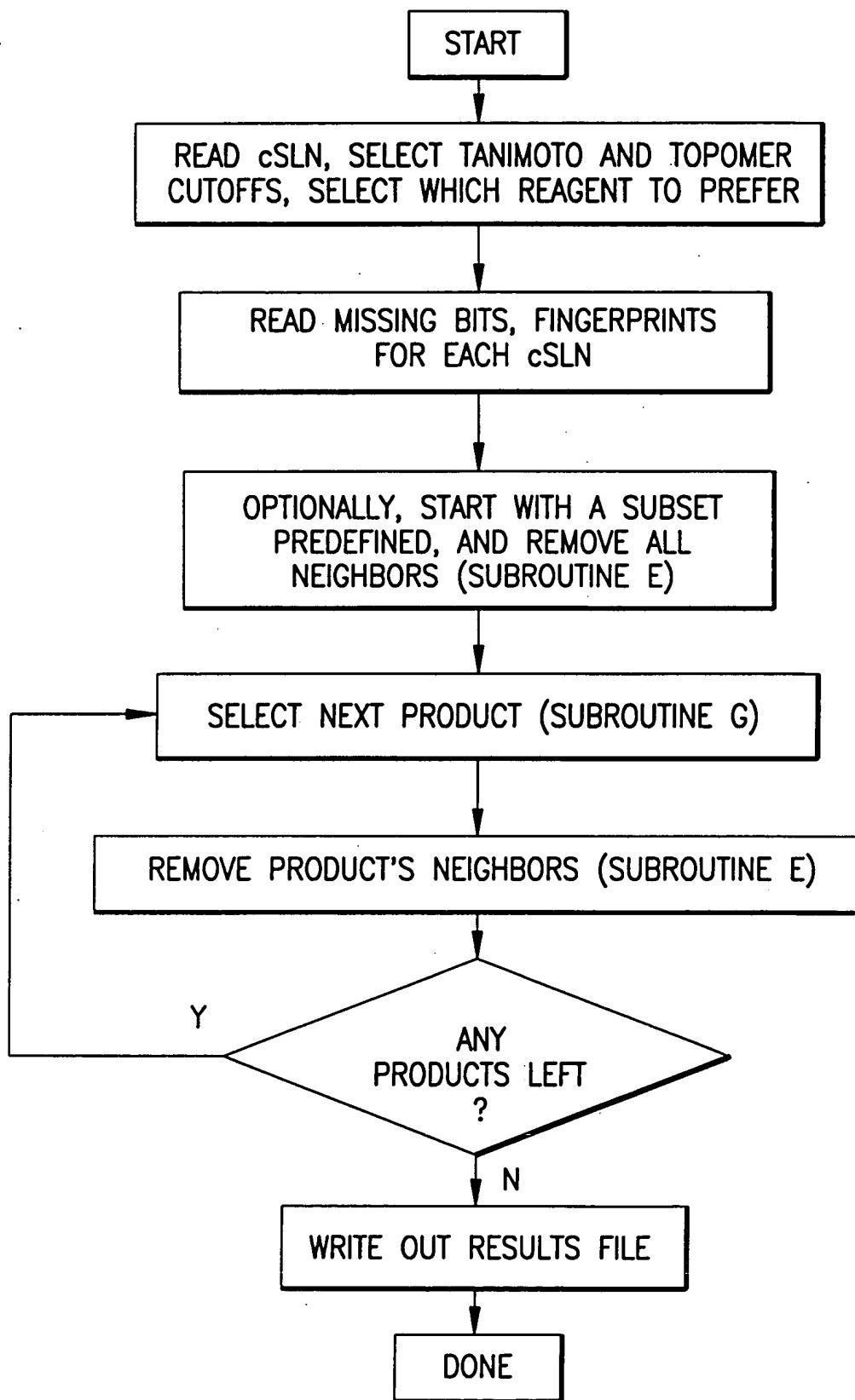


FIG.24

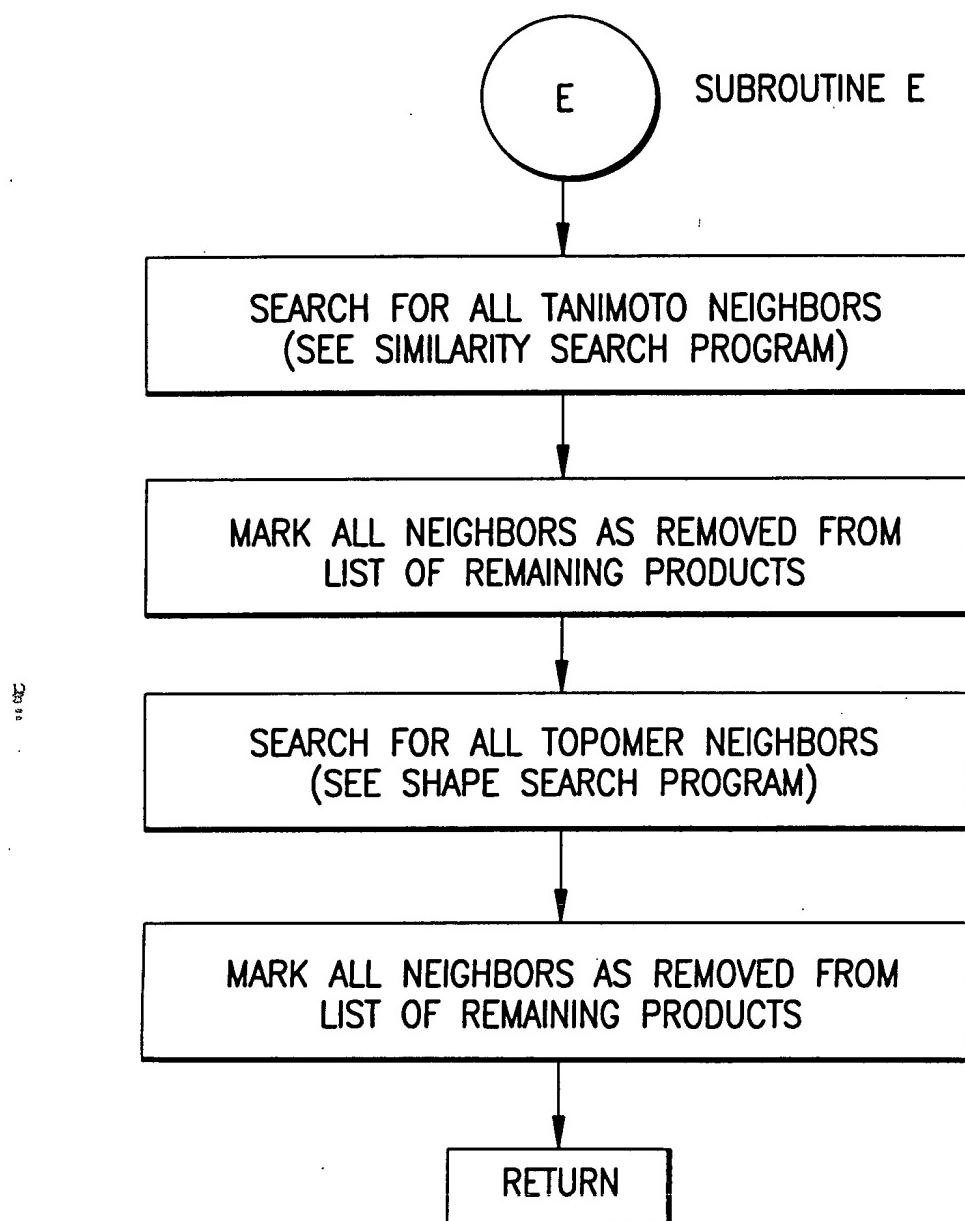


FIG.25

09866543 - 052504

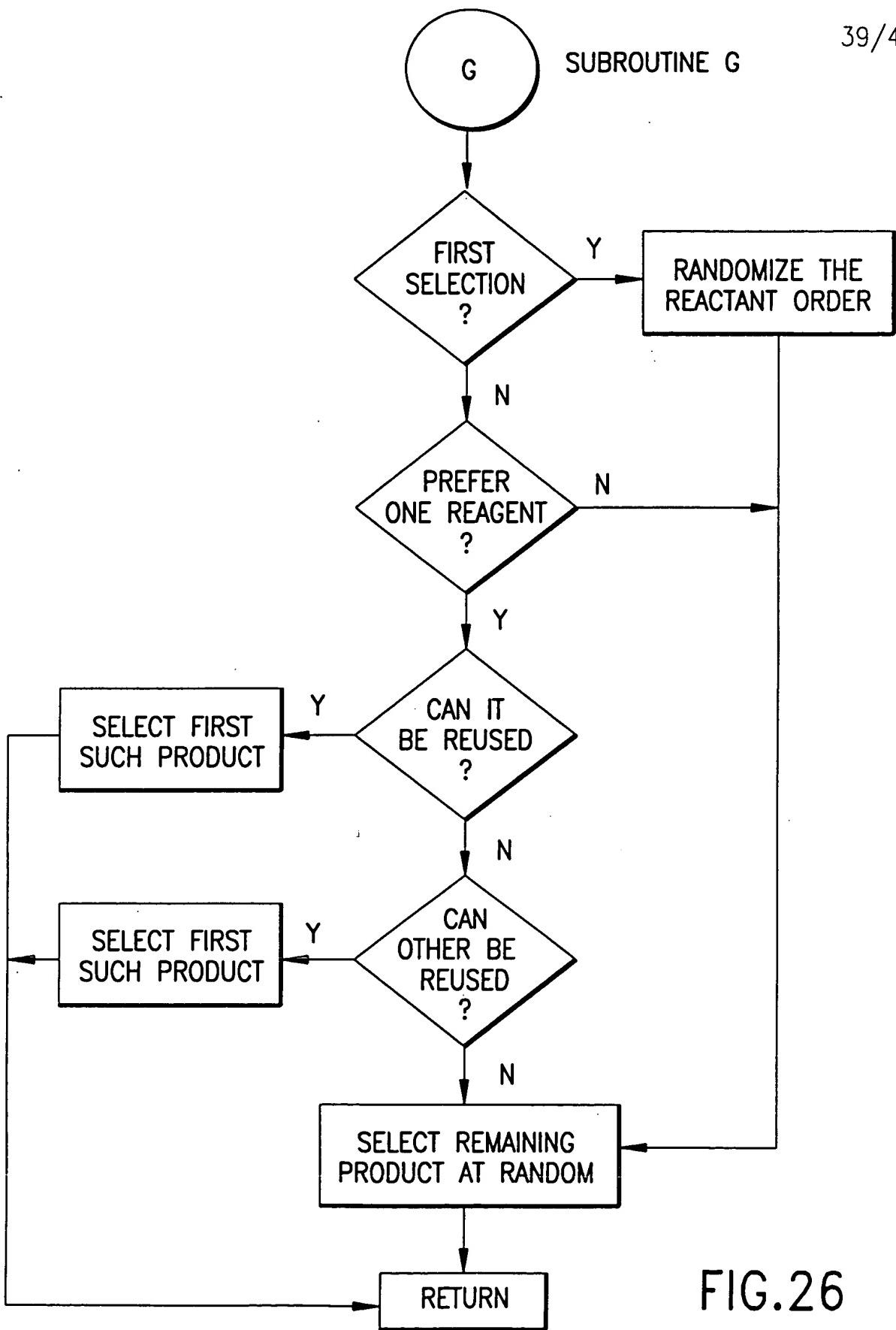


FIG.26

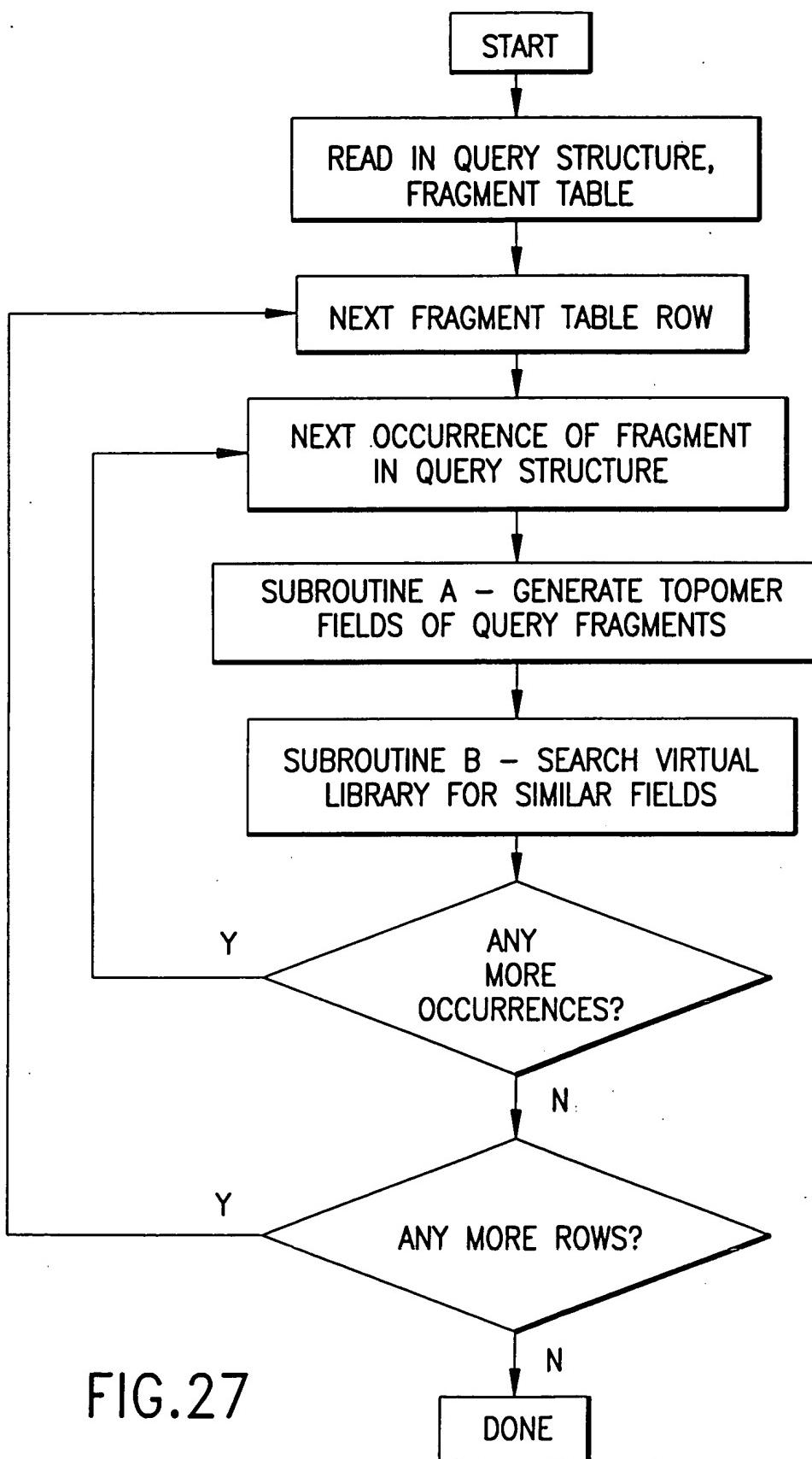


FIG.27

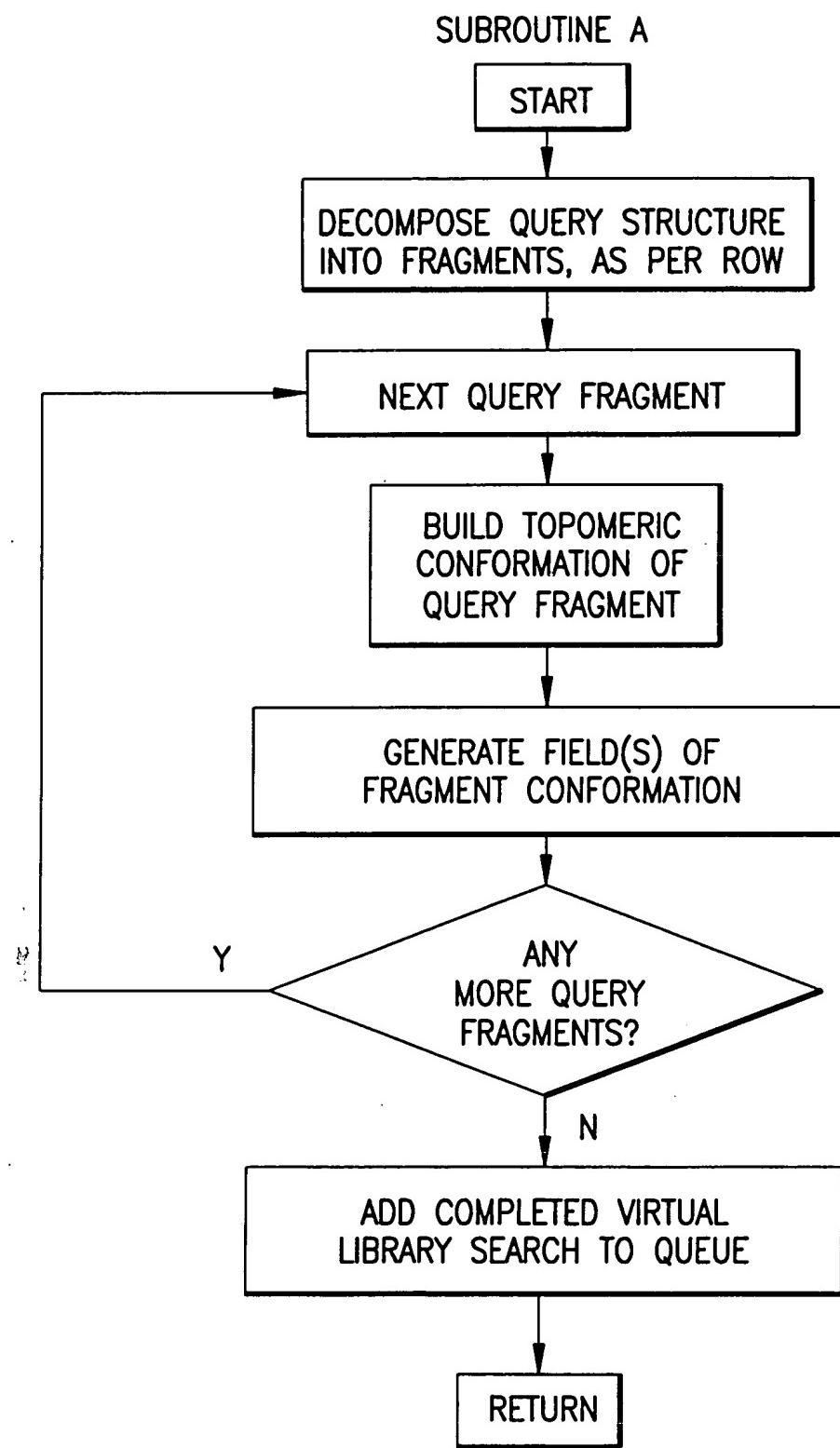
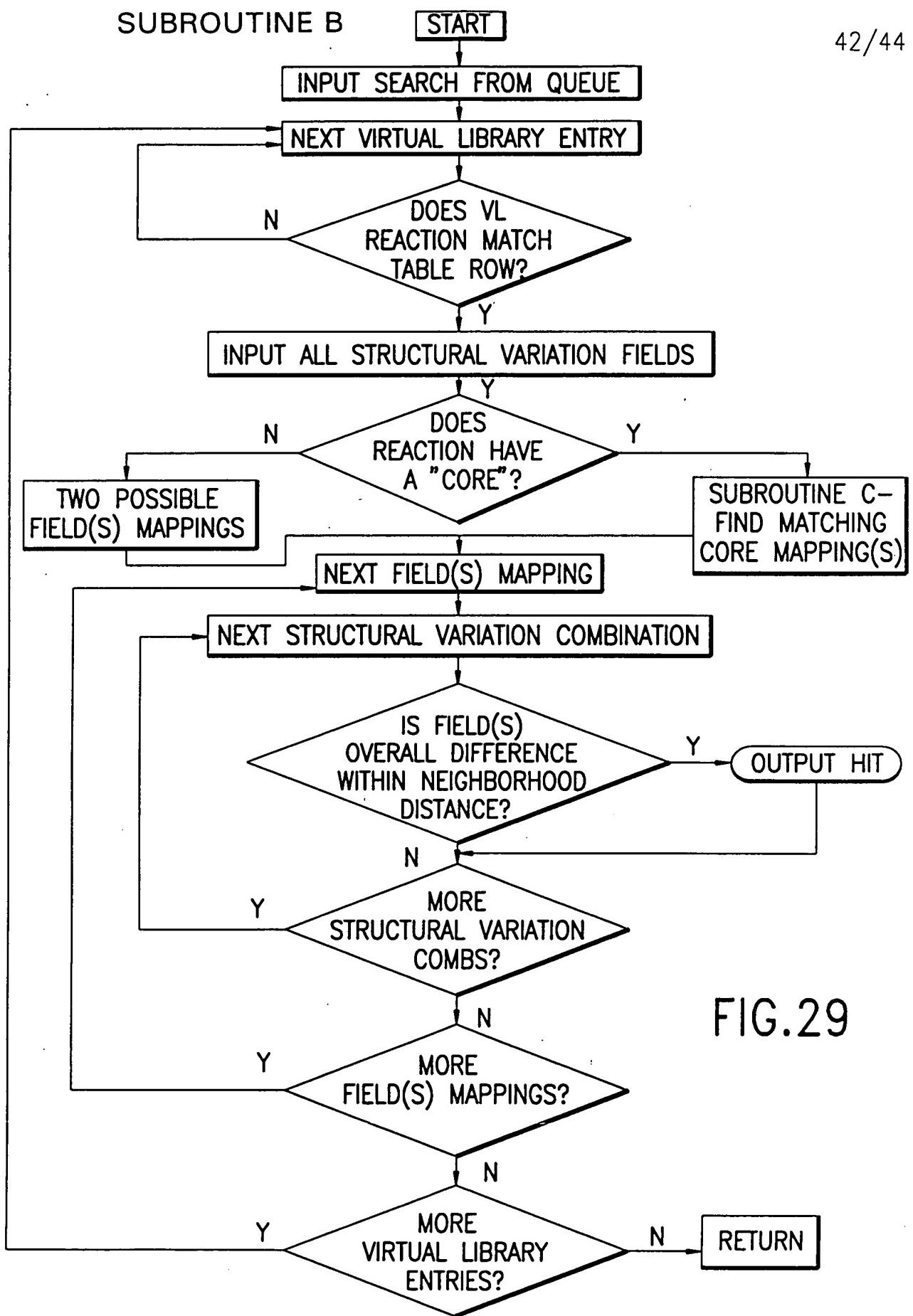


FIG.28

09866543 - 052504



098565543 - 052601

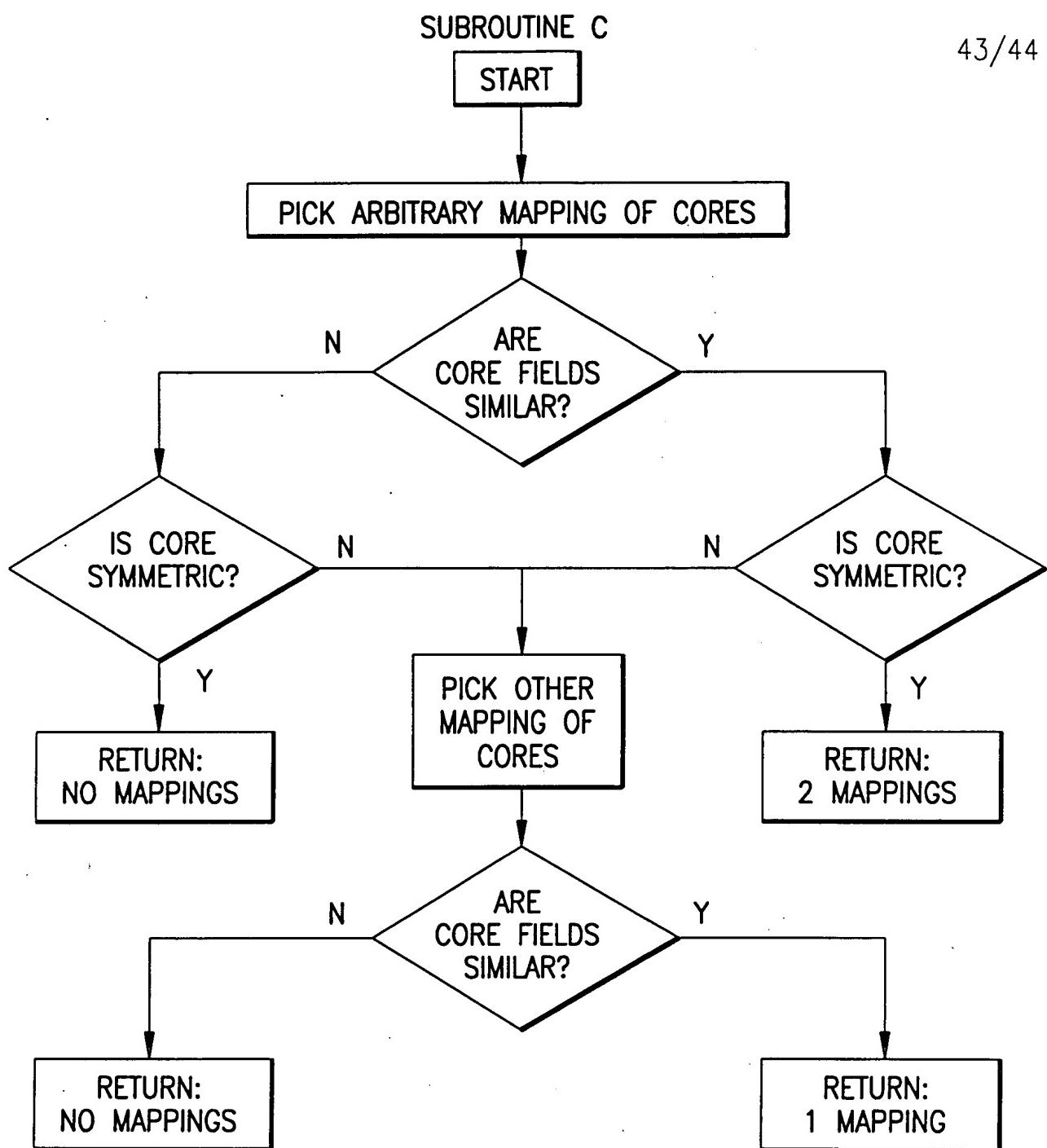


FIG.30

09866542 052604

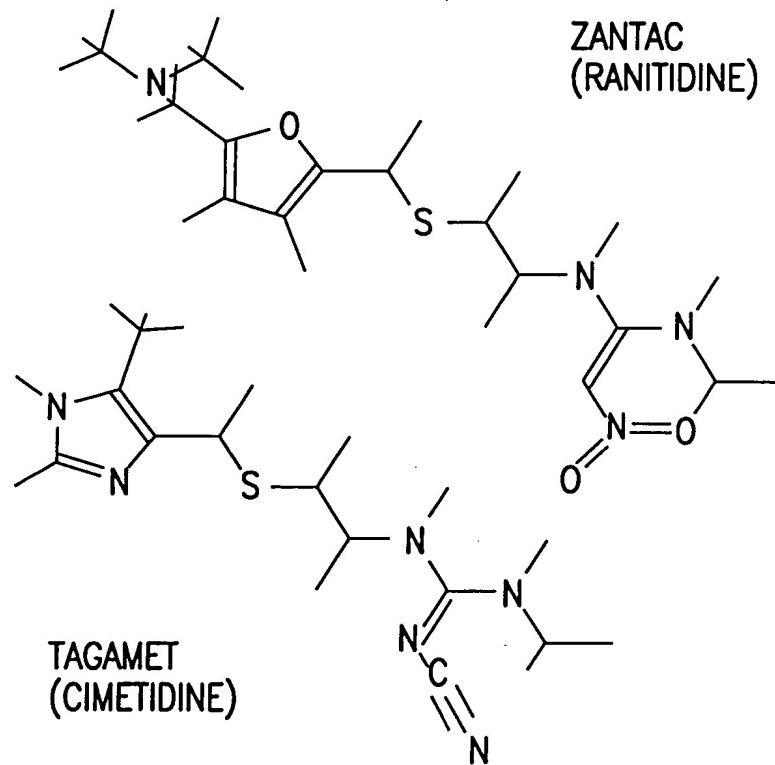


FIG.31